



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 07:30 PM EDT

PDB ID : 5J7L / pdb_00005j7l
Title : Structure of the 70S E coli ribosome with the U1052G mutation in the 16S rRNA bound to tetracycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-06
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

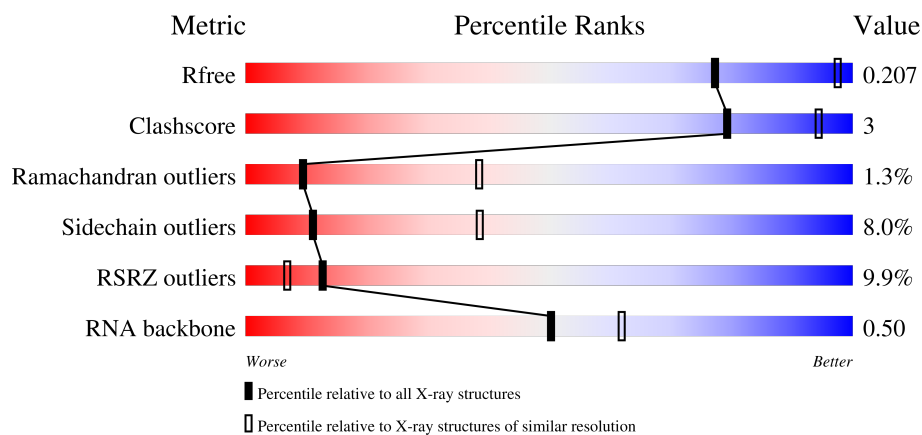
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	6% 75% 22% .
1	BA	1534	8% 74% 23% .
2	AB	224	4% 85% 12% .
2	BB	224	11% 86% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
30	DD	209	
31	CA	2904	
32	CE	201	
32	DE	201	
33	CF	177	
33	DF	177	
34	CG	176	
34	DG	176	
35	CH	149	
35	DH	149	
36	CJ	134	
36	DJ	134	
37	CK	142	
37	DK	142	
38	CL	123	
38	DL	123	
39	CM	144	
39	DM	144	
40	CN	136	
40	DN	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	CO	125	30% 80% 14% ...
41	DO	125	88% 10% ..
42	CP	117	14% 84% 14% ...
42	DP	117	% 82% 15% ..
43	CQ	114	11% 88% 11% .
43	DQ	114	% 88% 11% .
44	CR	117	26% 84% 16%
44	DR	117	89% 11%
45	CS	103	26% 78% 19% ..
45	DS	103	2% 88% 12%
46	CT	110	31% 82% 15% .
46	DT	110	% 85% 15% .
47	CU	93	38% 80% 15% 5%
47	DU	93	5% 86% 14%
48	CV	102	54% 77% 20% .
48	DV	102	% 82% 15% ..
49	CW	94	7% 84% 16%
49	DW	94	87% 13%
50	CX	76	16% 88% 11% .
50	DX	76	84% 13% .
51	CY	77	27% 79% 19% .
51	DY	77	% 86% 14%
52	CZ	62	31% 81% 19%
52	DZ	62	3% 89% 11%
53	DI	135	22% 71% 25% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	DA	2904	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1617	-	-	-	X
55	MG	AA	1622	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3135	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3148	-	-	-	X
58	PUT	AA	1674	-	-	-	X
66	ACY	DA	3196	-	X	-	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295261 atoms, of which 2 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 595593103
BA	1052	G	U	engineered mutation	GB 595593103

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
32	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
33	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
34	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
35	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			
36	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
37	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
38	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
39	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
40	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
41	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	CP	116	Total	C	N	O			
			892	552	178	162	0	0	0
42	DP	117	Total	C	N	O	S		
			900	557	179	163	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	CQ	114	Total	C	N	O	S		
			917	574	179	163	1	0	0
43	DQ	114	Total	C	N	O	S		
			917	574	179	163	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	CR	117	Total	C	N	O			
			947	604	192	151	0	0	0
44	DR	117	Total	C	N	O			
			947	604	192	151	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	CS	103	Total	C	N	O	S		
			816	516	153	145	2	0	0
45	DS	103	Total	C	N	O	S		
			816	516	153	145	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	CT	110	Total	C	N	O	S		
			857	532	166	156	3	0	0
46	DT	110	Total	C	N	O	S		
			857	532	166	156	3	0	0

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	CU	93	Total	C	N	O	S		
			739	466	139	132	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CV	102	Total	C	N	O		0	0	0
			780	492	146	142				
48	DV	102	Total	C	N	O		0	0	0
			780	492	146	142				

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
49	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 50 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
50	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
52	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

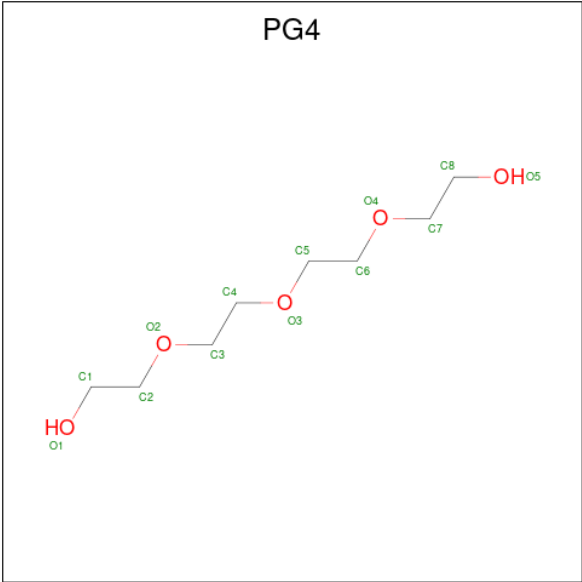
- Molecule 54 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

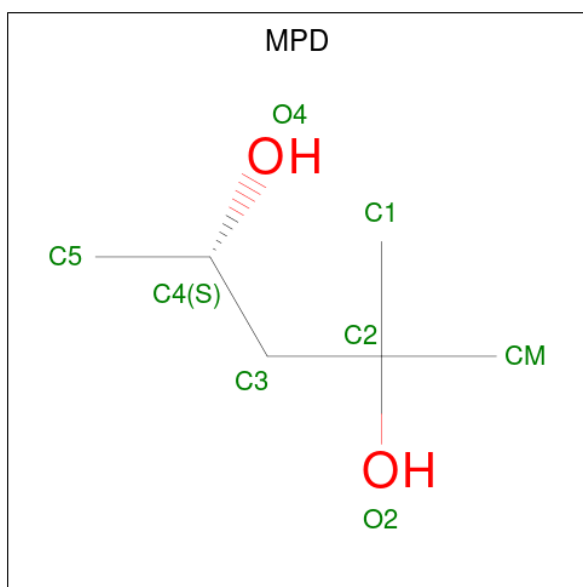
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total	Mg	0	0
			72	72		
55	BA	45	Total	Mg	0	0
			45	45		
55	CB	3	Total	Mg	0	0
			3	3		
55	CA	156	Total	Mg	0	0
			156	156		
55	DD	1	Total	Mg	0	0
			1	1		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	DB	9	Total	Mg	0	0
			9	9		
55	DA	183	Total	Mg	0	0
			183	183		

- Molecule 56 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



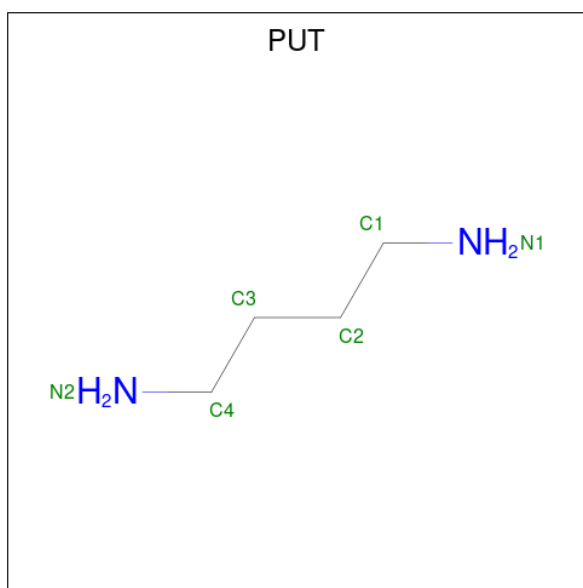
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		
56	DQ	1	Total	C	O	0	0
			13	8	5		
56	DR	1	Total	C	O	0	0
			13	8	5		
56	DS	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			8	6	2		
57	AA	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DK	1	Total	C	O	0	0
			8	6	2		
57	DN	1	Total	C	O	0	0
			8	6	2		
57	DS	1	Total	C	O	0	0
			8	6	2		
57	DT	1	Total	C	O	0	0
			8	6	2		
57	DT	1	Total	C	O	0	0
			8	6	2		
57	DA	1	Total	C	O	0	0
			8	6	2		
57	DA	1	Total	C	O	0	0
			8	6	2		
57	DA	1	Total	C	O	0	0
			8	6	2		
57	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



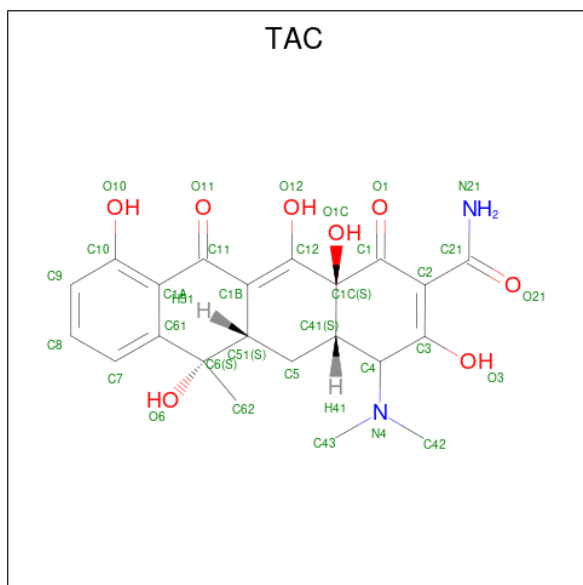
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	DM	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0

- Molecule 59 is TETRACYCLINE (CCD ID: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AA	1	Total 32	C 22	N 2	O 8	0	0	
59	AA	1	Total 33	C 22	H 1	N 2	O 8	0	0
59	BA	1	Total 32	C 22	N 2	O 8	0	0	
59	BA	1	Total 33	C 22	H 1	N 2	O 8	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

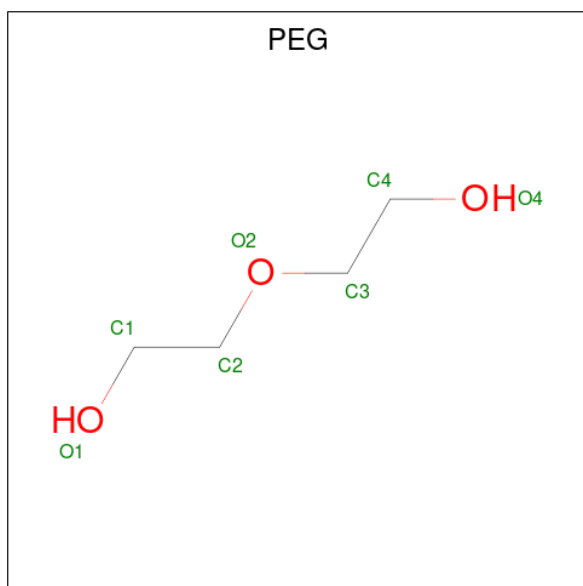
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AB	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	D5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



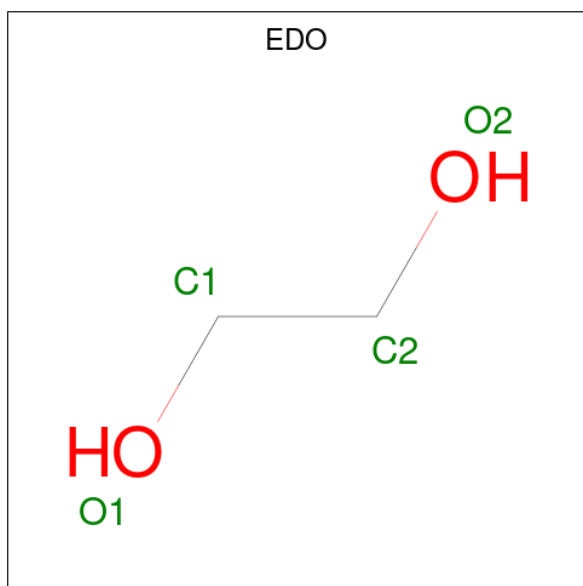
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DA	1	Total	C	O	0	0
			7	4	3		

- Molecule 62 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



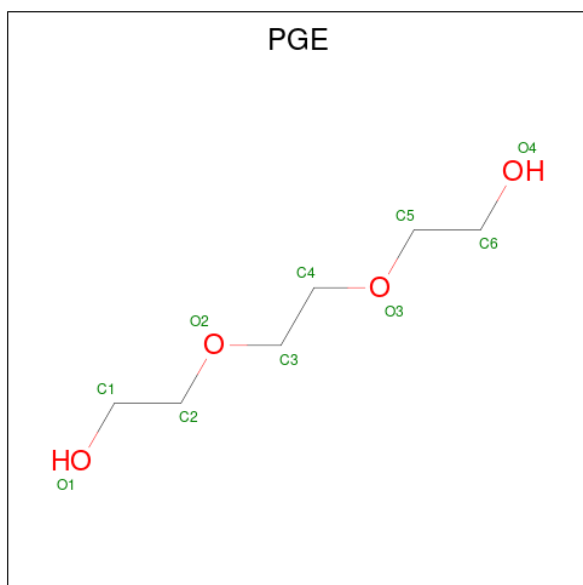
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

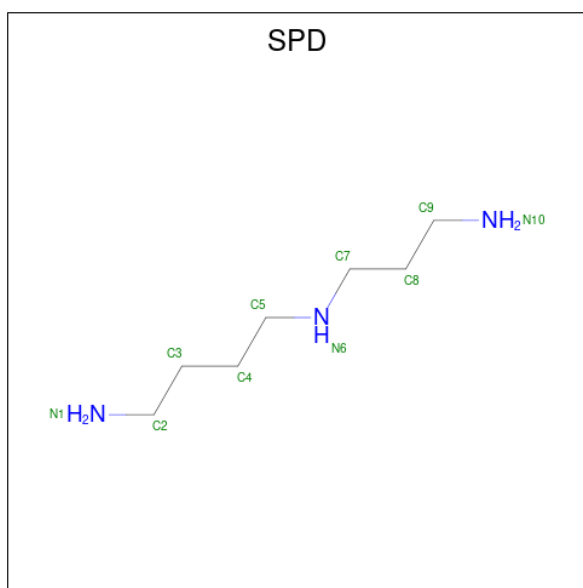
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



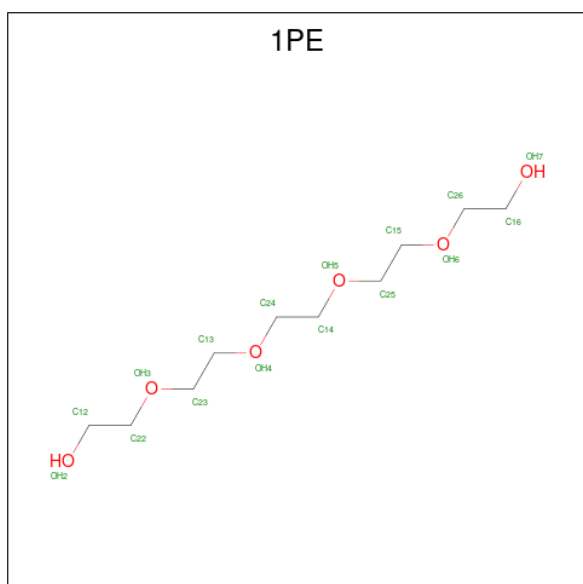
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



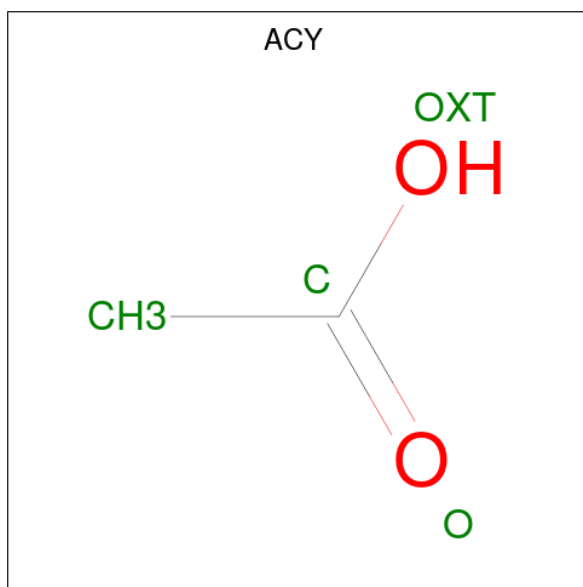
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



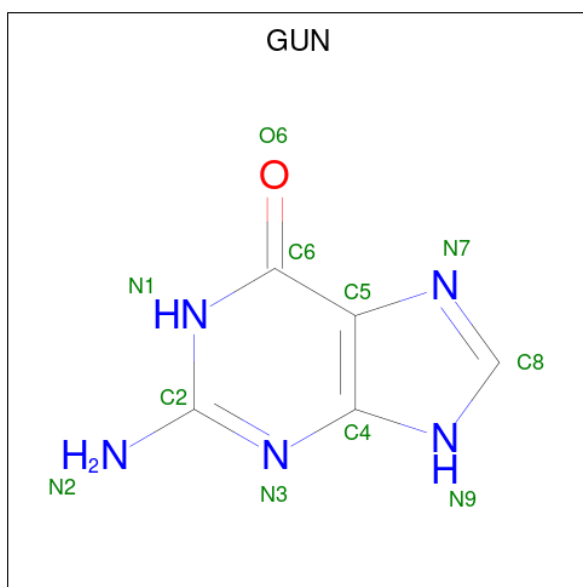
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



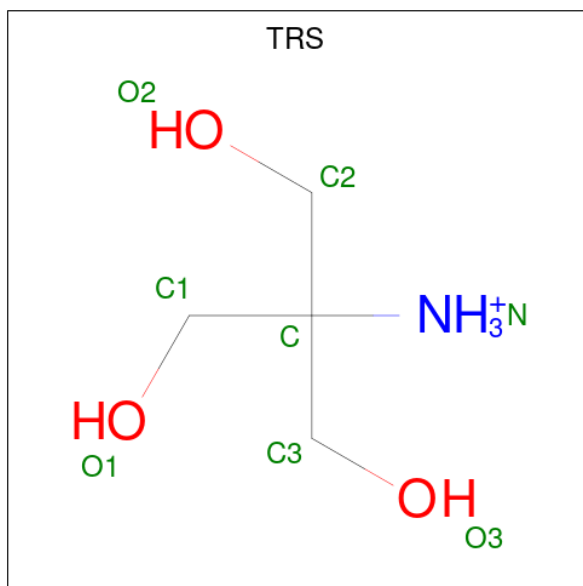
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
67	DA	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	501	Total 501	O 501	0	0
69	AC	4	Total 4	O 4	0	0
69	AD	2	Total 2	O 2	0	0
69	AE	5	Total 5	O 5	0	0
69	AG	1	Total 1	O 1	0	0
69	AH	1	Total 1	O 1	0	0
69	AJ	2	Total 2	O 2	0	0
69	AK	6	Total 6	O 6	0	0
69	AL	10	Total 10	O 10	0	0
69	AM	5	Total 5	O 5	0	0
69	AN	6	Total 6	O 6	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AR	1	Total 1	O 1	0	0
69	AT	3	Total 3	O 3	0	0
69	AU	3	Total 3	O 3	0	0
69	C3	4	Total 4	O 4	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	13	Total 13	O 13	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BK	2	Total	O	0	0
			2	2		
69	BL	4	Total	O	0	0
			4	4		
69	BN	2	Total	O	0	0
			2	2		
69	BO	1	Total	O	0	0
			1	1		
69	BP	3	Total	O	0	0
			3	3		
69	BT	2	Total	O	0	0
			2	2		
69	BU	2	Total	O	0	0
			2	2		
69	D1	43	Total	O	0	0
			43	43		
69	D2	6	Total	O	0	0
			6	6		
69	D3	22	Total	O	0	0
			22	22		
69	D4	39	Total	O	0	0
			39	39		
69	D5	8	Total	O	0	0
			8	8		
69	D0	24	Total	O	0	0
			24	24		
69	CB	13	Total	O	0	0
			13	13		
69	CC	10	Total	O	0	0
			10	10		
69	CD	6	Total	O	0	0
			6	6		
69	CA	691	Total	O	0	0
			691	691		
69	DC	100	Total	O	0	0
			100	100		
69	DD	98	Total	O	0	0
			98	98		
69	CE	5	Total	O	0	0
			5	5		
69	CL	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CM	4	Total	O	0	0
			4	4		
69	CO	2	Total	O	0	0
			2	2		
69	CU	3	Total	O	0	0
			3	3		
69	CV	1	Total	O	0	0
			1	1		
69	CW	1	Total	O	0	0
			1	1		
69	CY	1	Total	O	0	0
			1	1		
69	DE	61	Total	O	0	0
			61	61		
69	DF	15	Total	O	0	0
			15	15		
69	DG	6	Total	O	0	0
			6	6		
69	DH	2	Total	O	0	0
			2	2		
69	DK	65	Total	O	0	0
			65	65		
69	DL	52	Total	O	0	0
			52	52		
69	DM	63	Total	O	0	0
			63	63		
69	DN	72	Total	O	0	0
			72	72		
69	DO	44	Total	O	0	0
			44	44		
69	DP	38	Total	O	0	0
			38	38		
69	DQ	33	Total	O	0	0
			33	33		
69	DR	62	Total	O	0	0
			62	62		
69	DS	46	Total	O	0	0
			46	46		
69	DT	69	Total	O	0	0
			69	69		
69	DU	18	Total	O	0	0
			18	18		

Continued on next page...

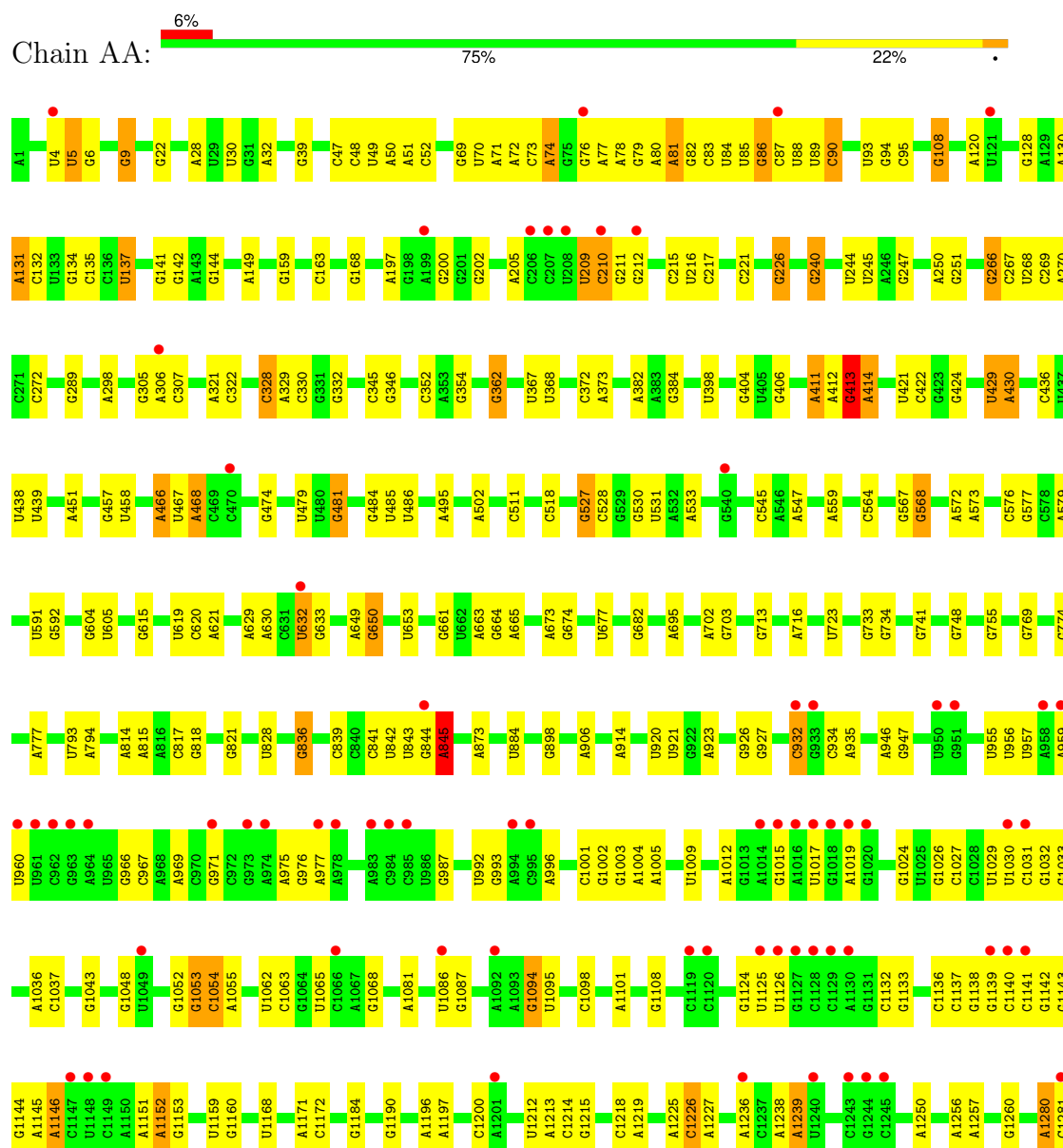
Continued from previous page...

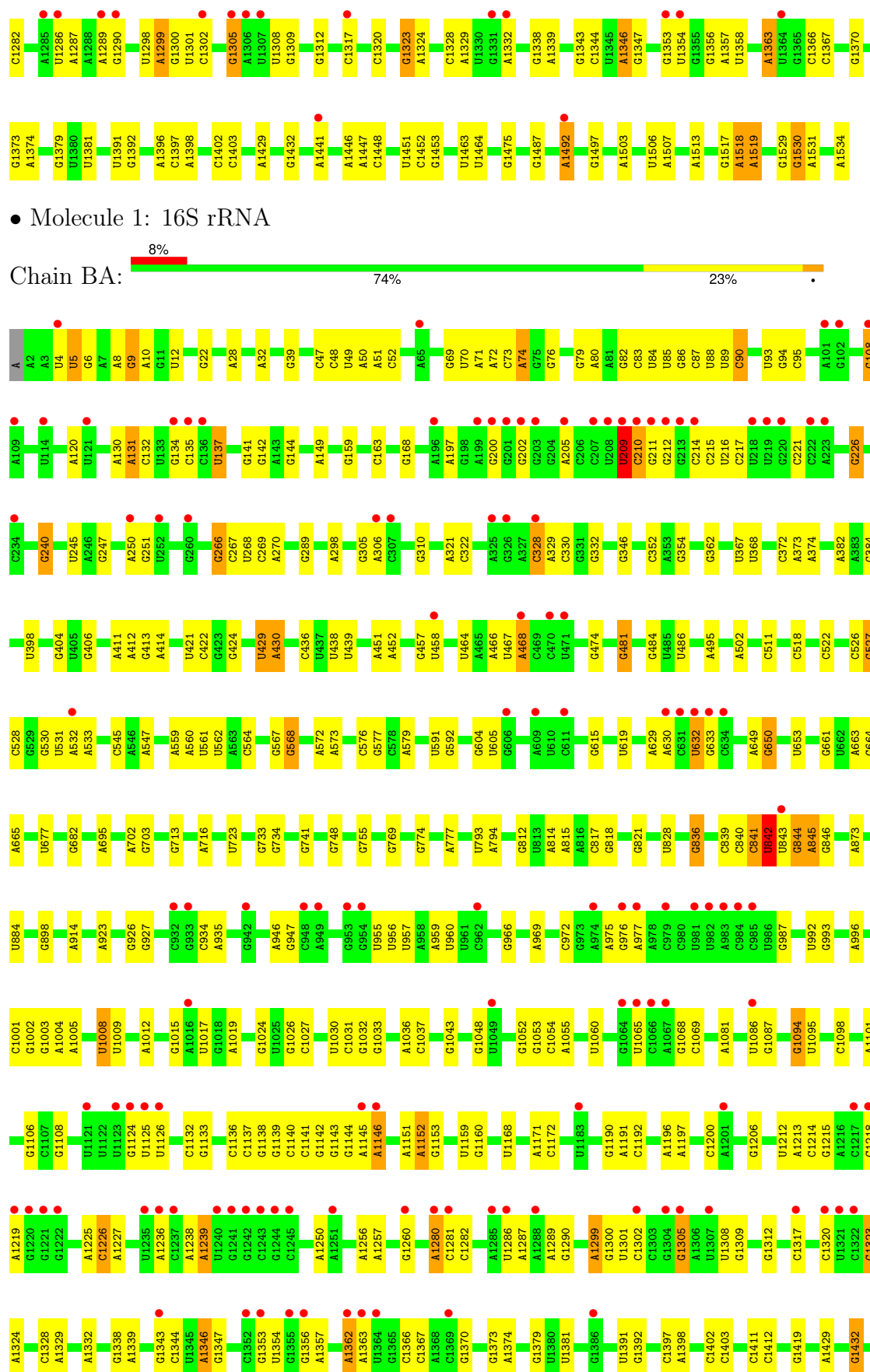
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DV	20	Total 20	O 20	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	25	Total 25	O 25	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	8	Total 8	O 8	0	0
69	DB	209	Total 209	O 209	0	0
69	DA	4840	Total 4840	O 4840	0	0

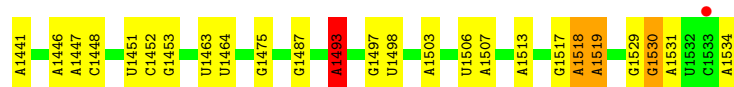
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

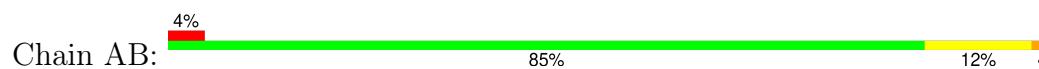
• Molecule 1: 16S rRNA



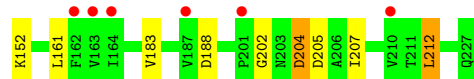
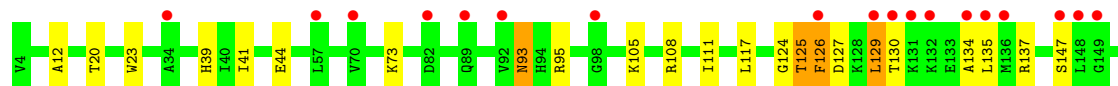
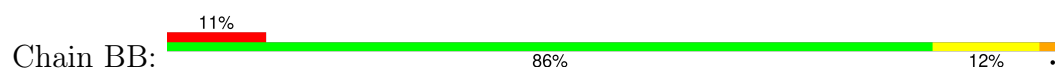




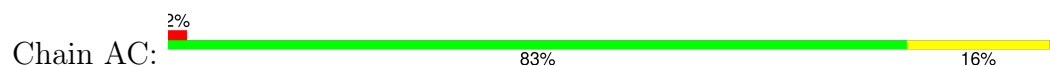
- Molecule 2: 30S ribosomal protein S2



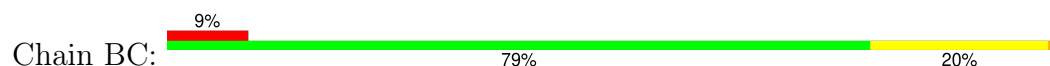
- Molecule 2: 30S ribosomal protein S2



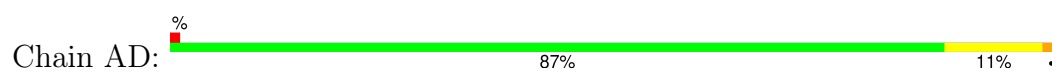
- Molecule 3: 30S ribosomal protein S3



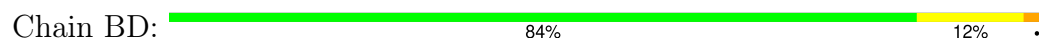
- Molecule 3: 30S ribosomal protein S3



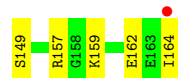
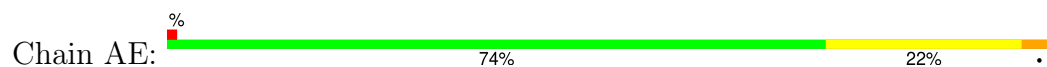
- Molecule 4: 30S ribosomal protein S4



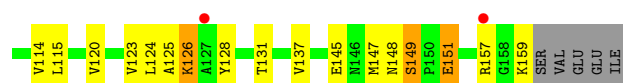
- Molecule 4: 30S ribosomal protein S4



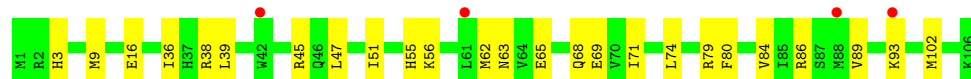
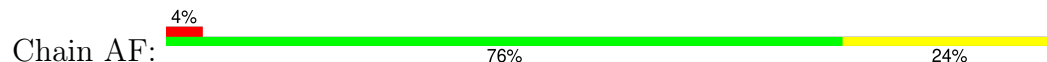
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



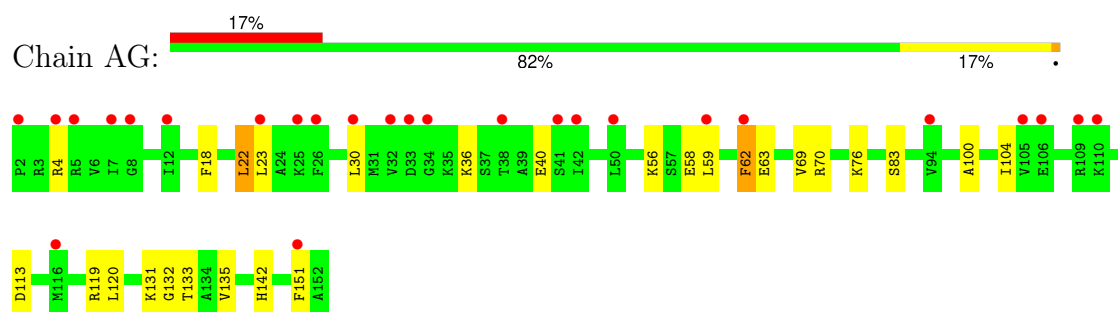
- Molecule 6: 30S ribosomal protein S6



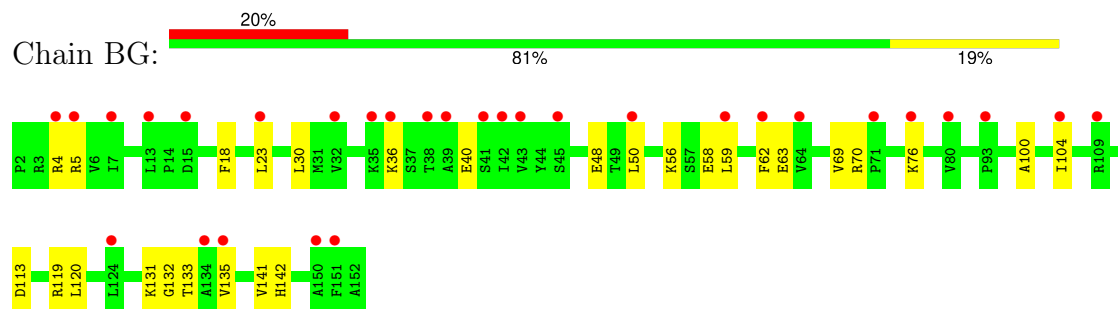
- Molecule 6: 30S ribosomal protein S6



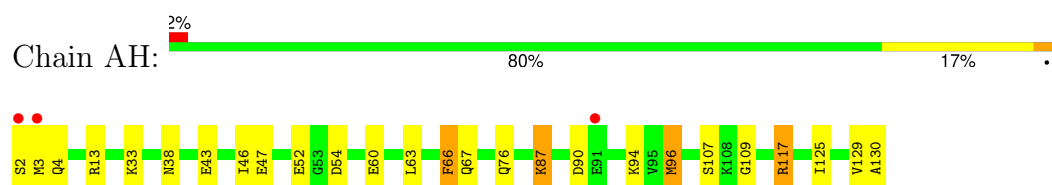
- Molecule 7: 30S ribosomal protein S7



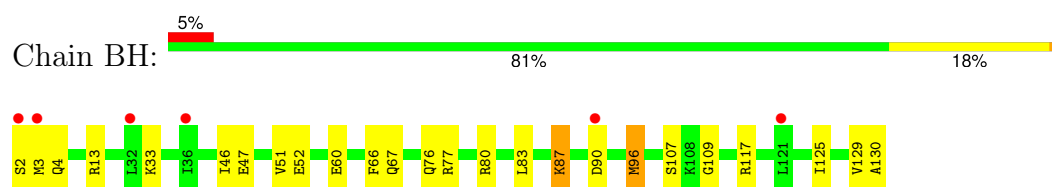
- Molecule 7: 30S ribosomal protein S7



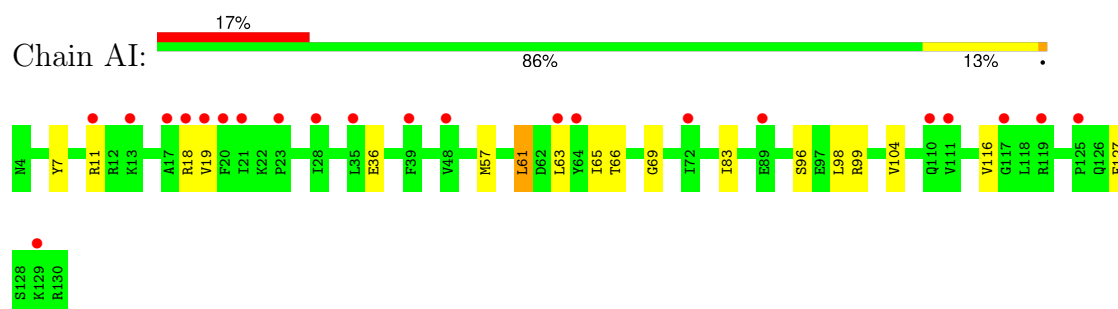
- Molecule 8: 30S ribosomal protein S8



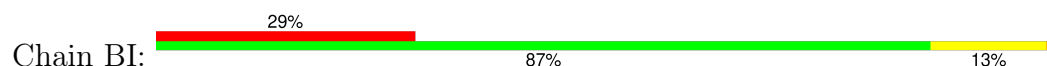
- Molecule 8: 30S ribosomal protein S8

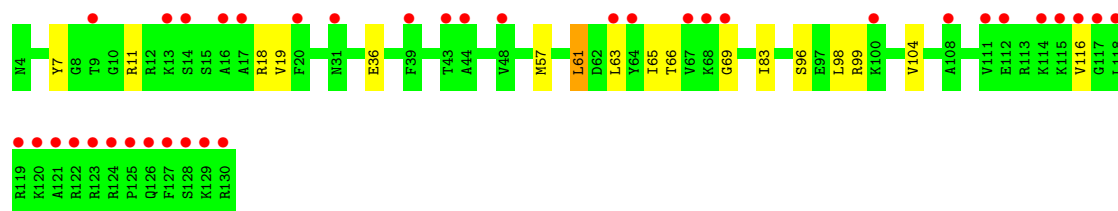


- Molecule 9: 30S ribosomal protein S9

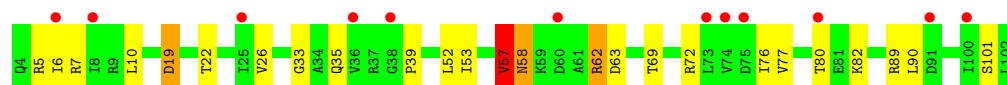
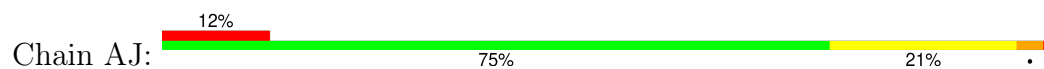


- Molecule 9: 30S ribosomal protein S9

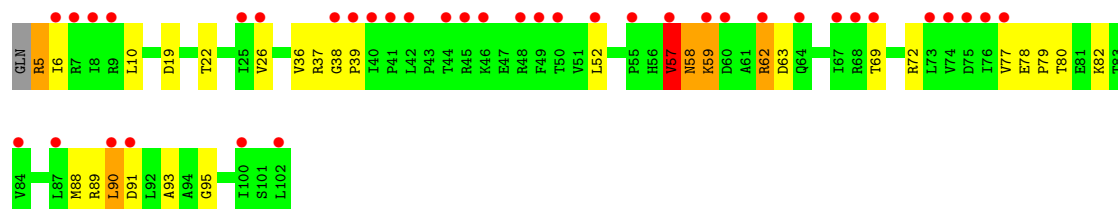
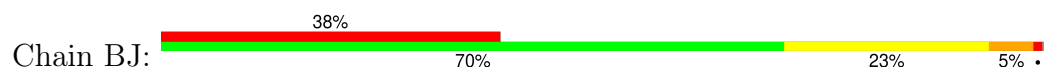




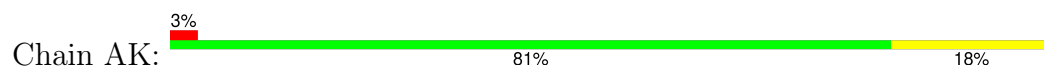
- Molecule 10: 30S ribosomal protein S10



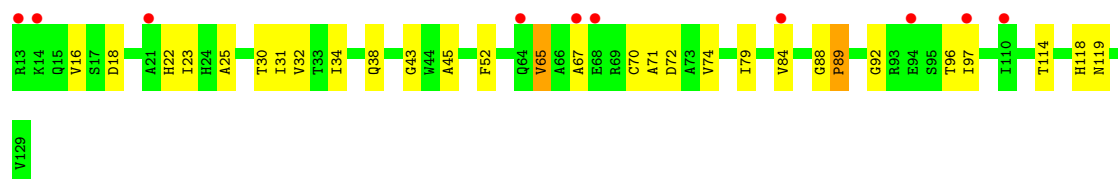
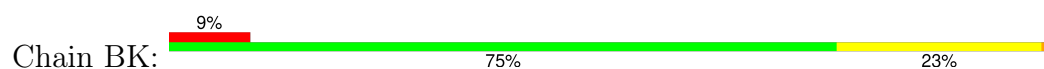
- Molecule 10: 30S ribosomal protein S10



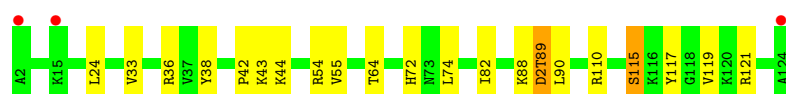
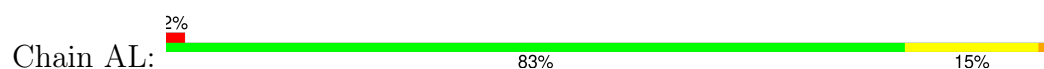
- Molecule 11: 30S ribosomal protein S11



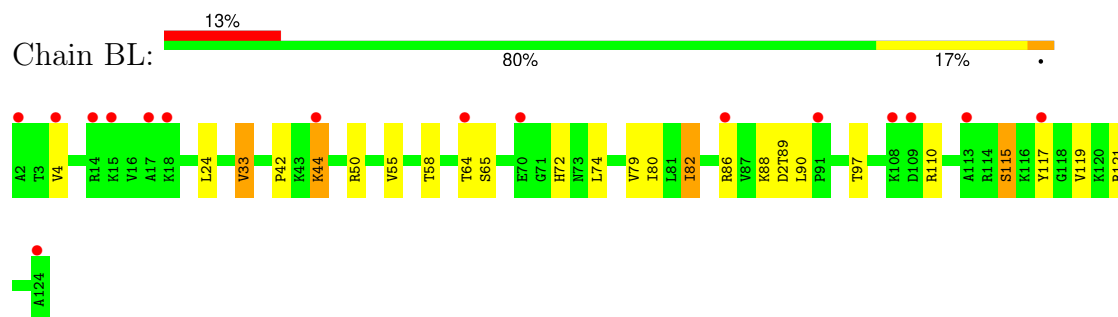
- Molecule 11: 30S ribosomal protein S11



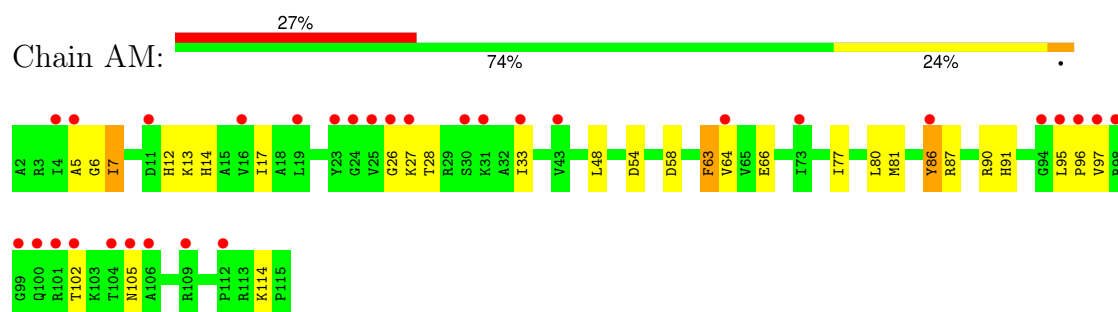
- Molecule 12: 30S ribosomal protein S12



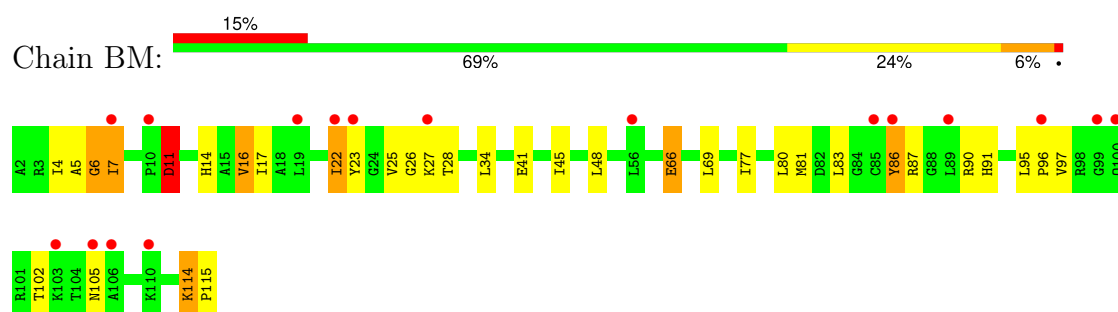
- Molecule 12: 30S ribosomal protein S12



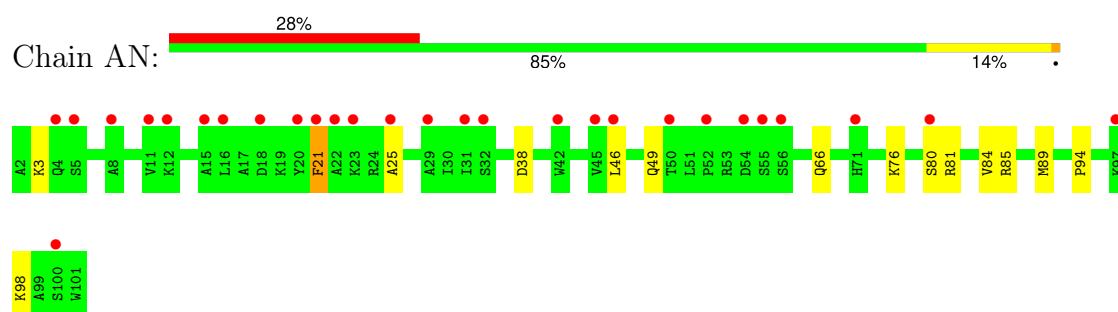
- Molecule 13: 30S ribosomal protein S13



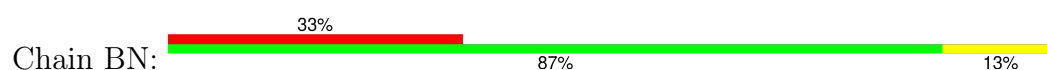
- Molecule 13: 30S ribosomal protein S13

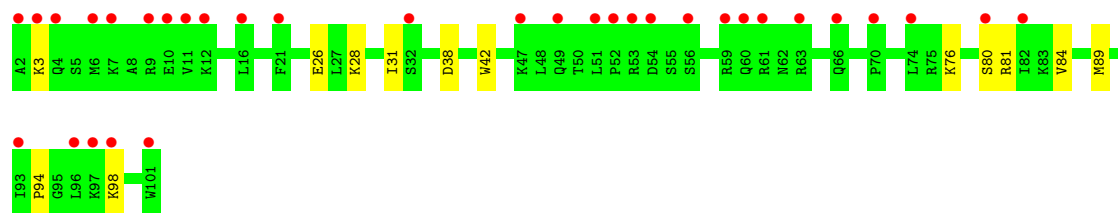


- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

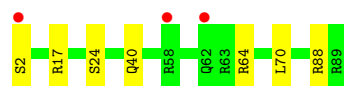




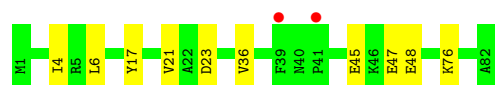
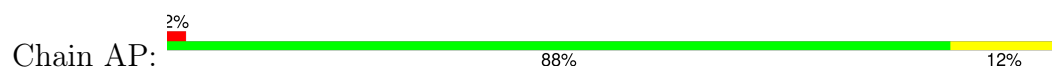
- Molecule 15: 30S ribosomal protein S15



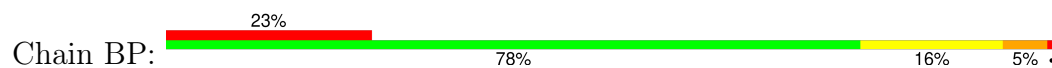
- Molecule 15: 30S ribosomal protein S15



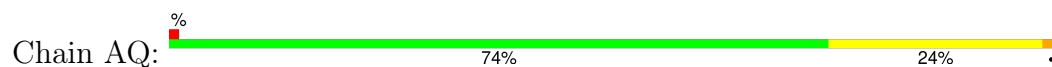
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

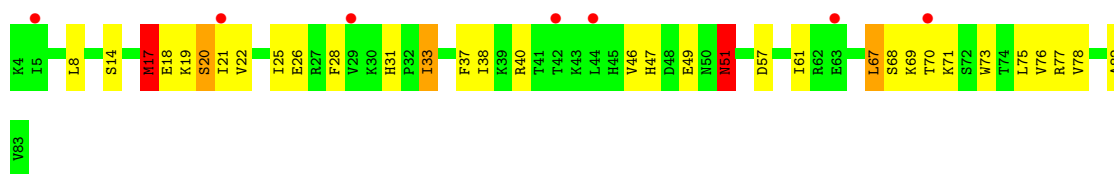


- Molecule 17: 30S ribosomal protein S17

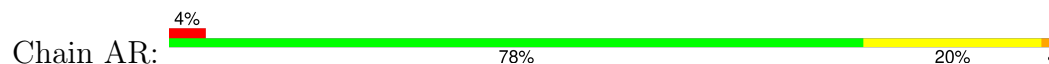


- Molecule 17: 30S ribosomal protein S17

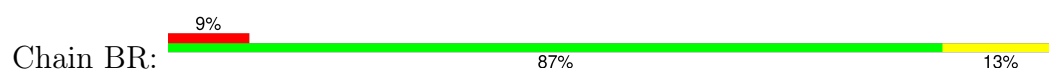




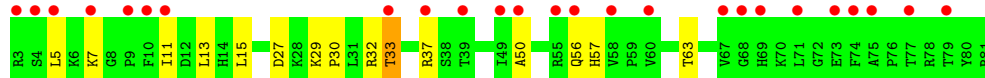
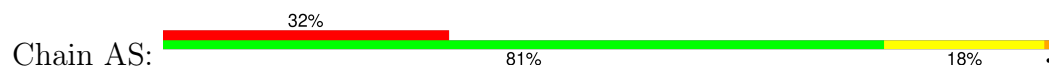
- Molecule 18: 30S ribosomal protein S18



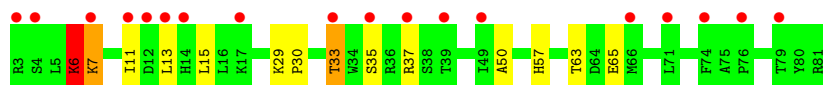
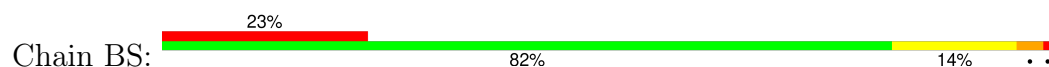
- Molecule 18: 30S ribosomal protein S18



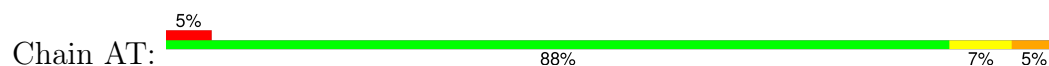
- Molecule 19: 30S ribosomal protein S19



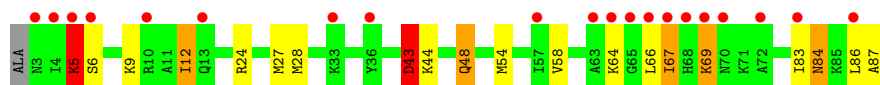
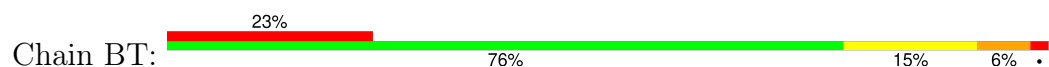
- Molecule 19: 30S ribosomal protein S19



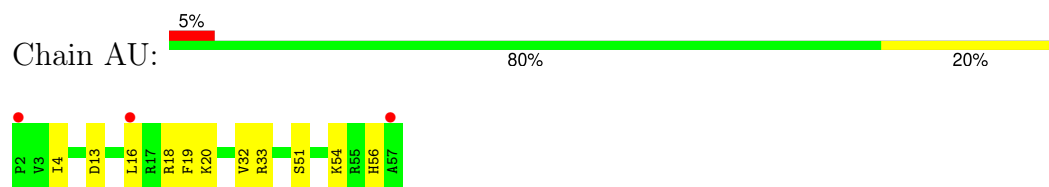
- Molecule 20: 30S ribosomal protein S20



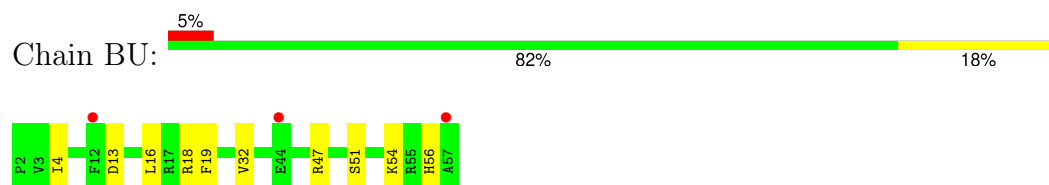
- Molecule 20: 30S ribosomal protein S20



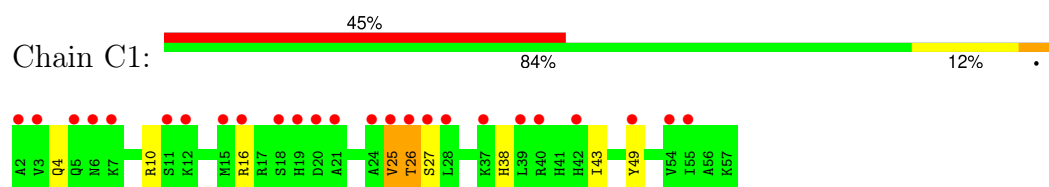
- Molecule 21: 30S ribosomal protein S21



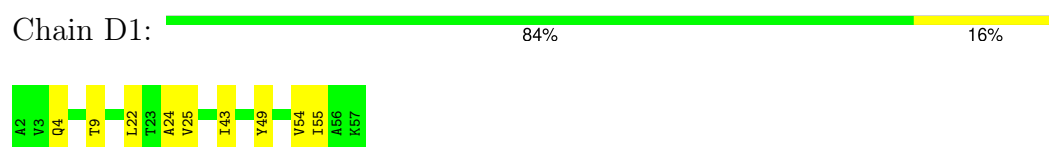
- Molecule 21: 30S ribosomal protein S21



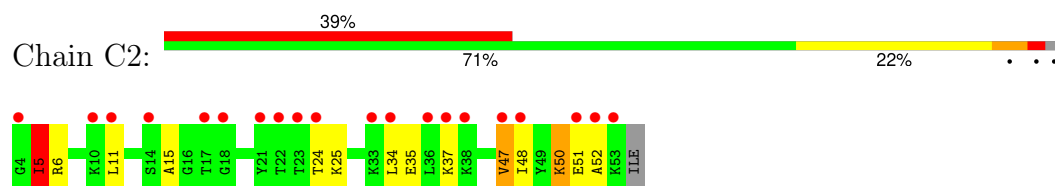
- Molecule 22: 50S ribosomal protein L32



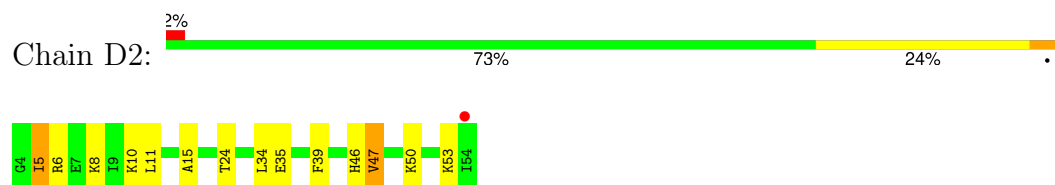
- Molecule 22: 50S ribosomal protein L32



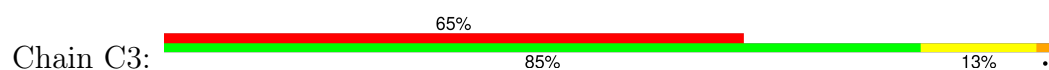
- Molecule 23: 50S ribosomal protein L33

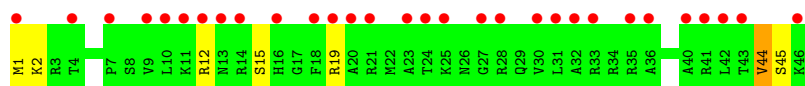


- Molecule 23: 50S ribosomal protein L33

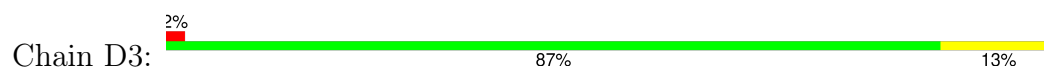


- Molecule 24: 50S ribosomal protein L34

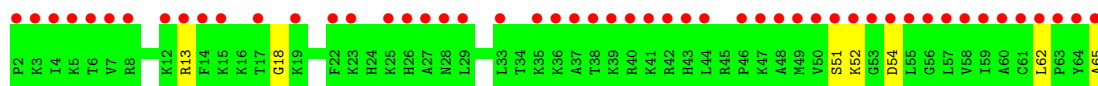
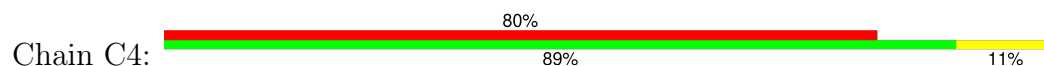




- Molecule 24: 50S ribosomal protein L34



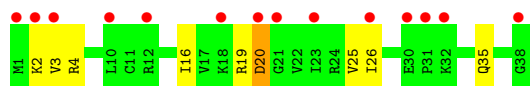
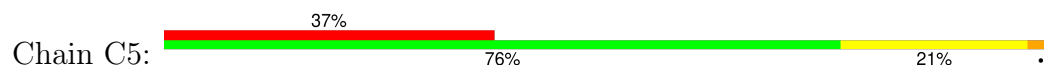
- Molecule 25: 50S ribosomal protein L35



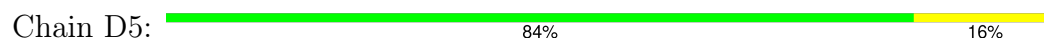
- Molecule 25: 50S ribosomal protein L35



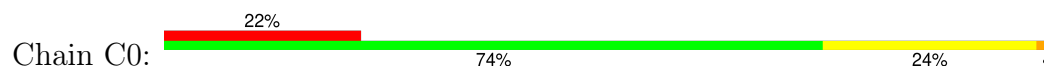
- Molecule 26: 50S ribosomal protein L36



- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30

Chain D0:  83% 16% .



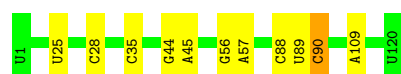
- Molecule 28: 5S rRNA

Chain CB:  3% 85% 11% . .



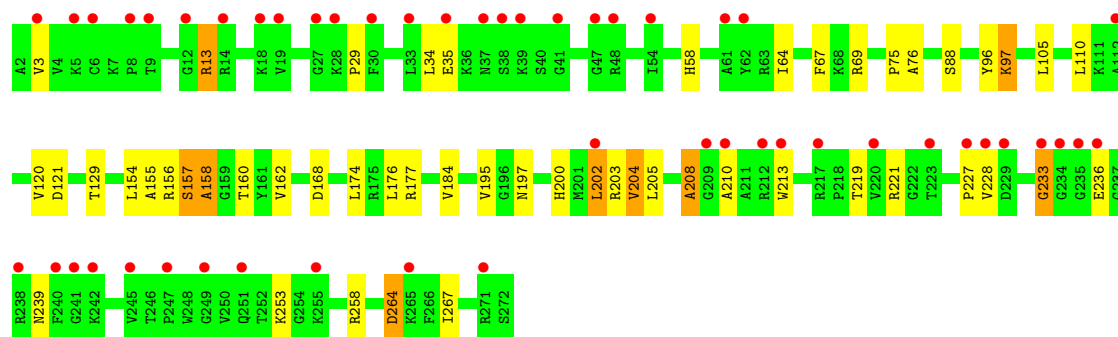
- Molecule 28: 5S rRNA

Chain DB:  91% 8% .



- Molecule 29: 50S ribosomal protein L2

Chain CC:  18% 81% 16% .



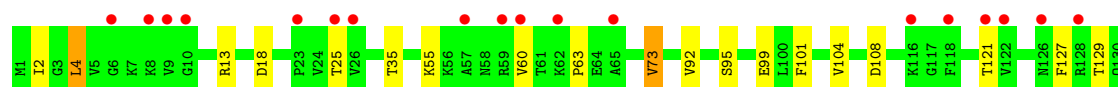
- Molecule 29: 50S ribosomal protein L2

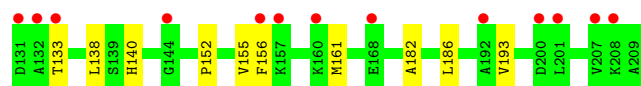
Chain DC:  89% 9% .



- Molecule 30: 50S ribosomal protein L3

Chain CD:  15% 86% 13% .





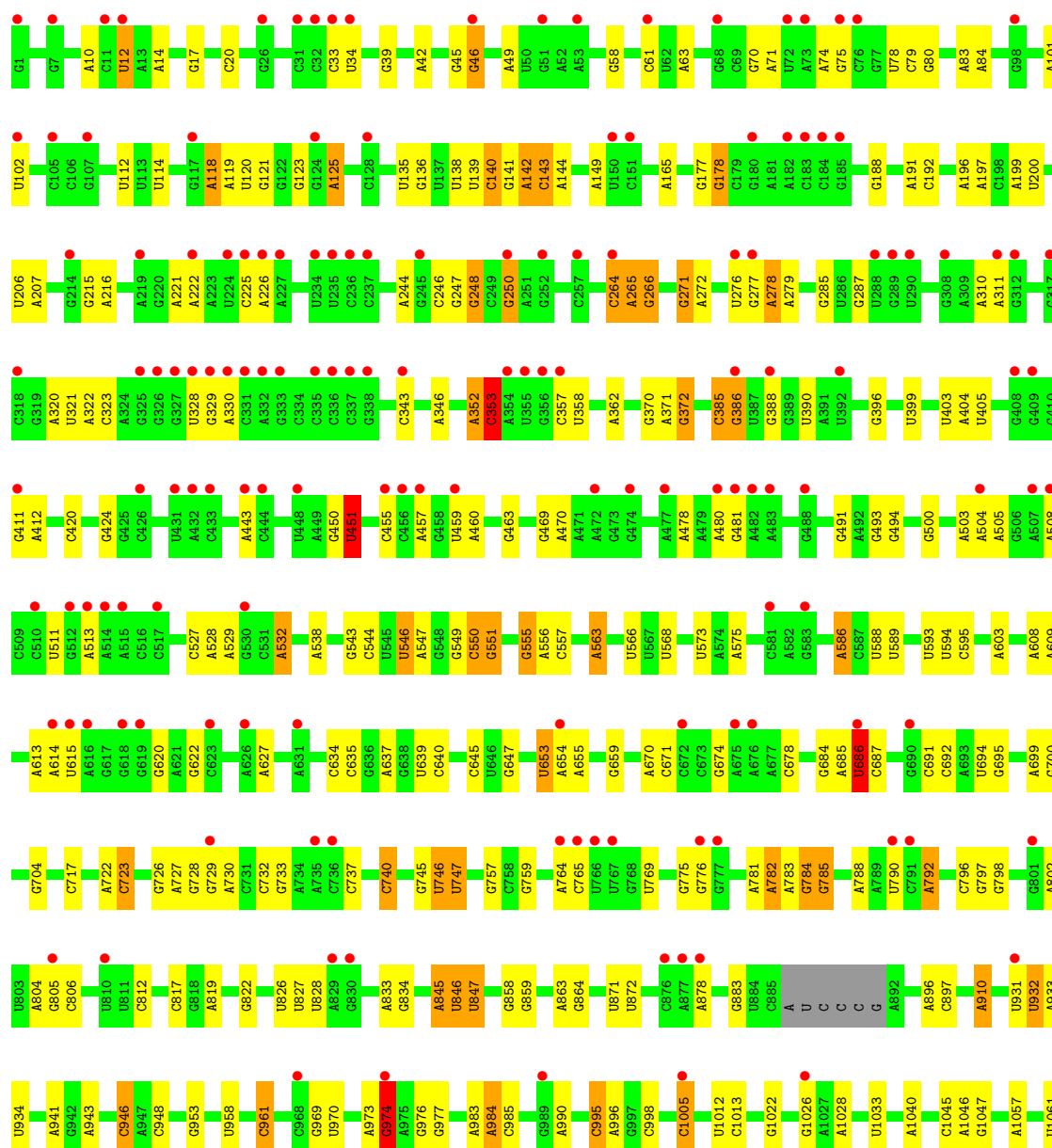
- Molecule 30: 50S ribosomal protein L3

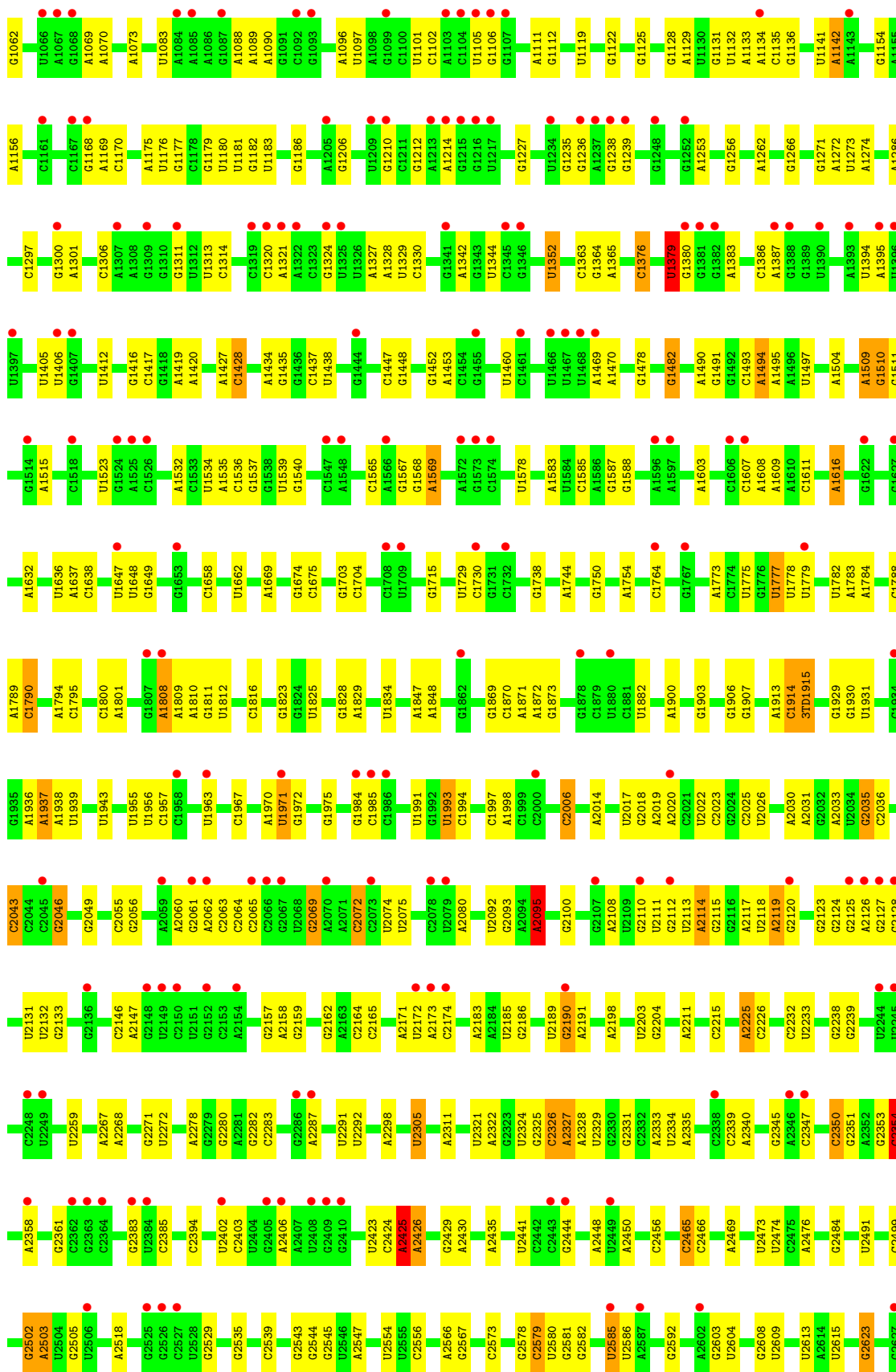
Chain DD: 88% 11% .

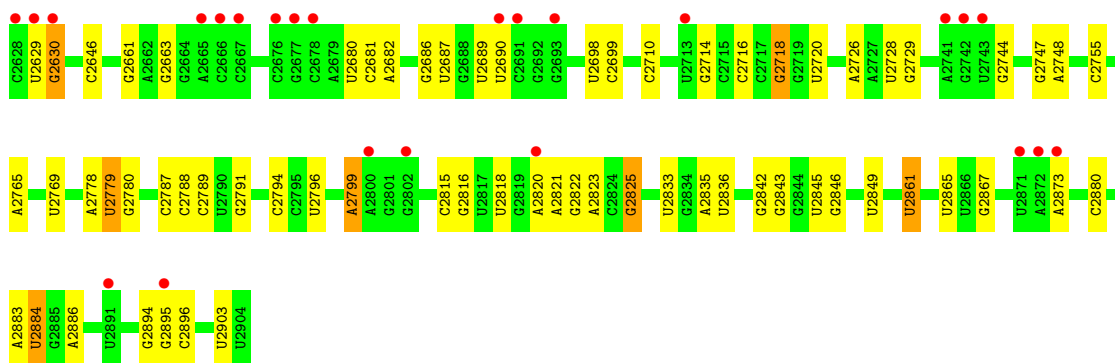


- Molecule 31: 23S rRNA

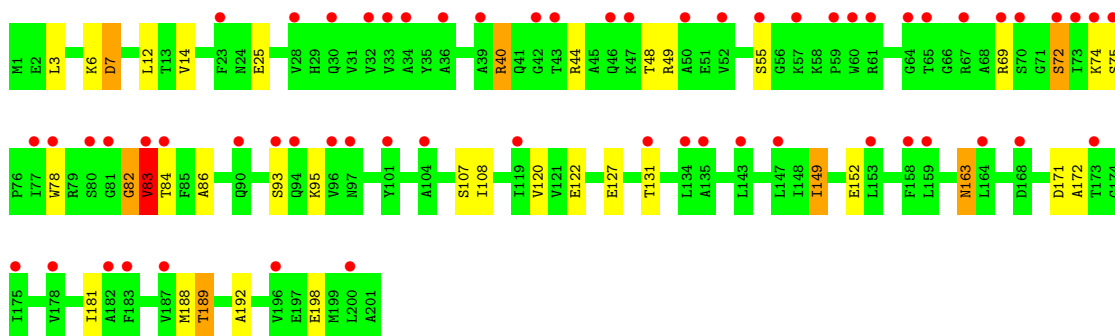
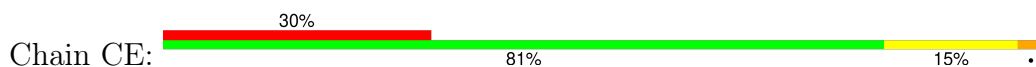
Chain CA: 12% 73% 23% .



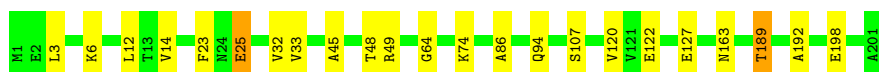




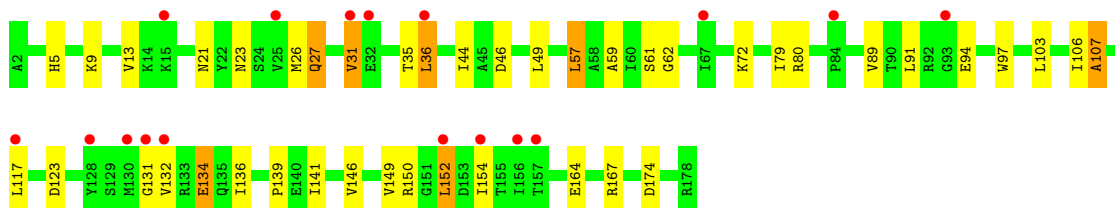
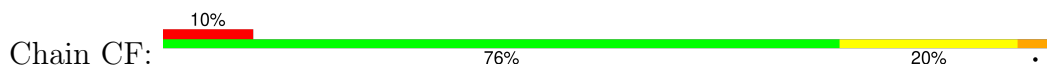
- Molecule 32: 50S ribosomal protein L4



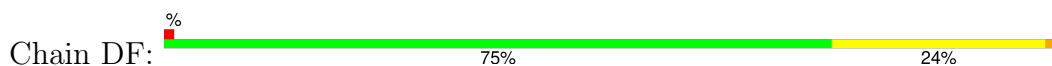
- Molecule 32: 50S ribosomal protein L4



- Molecule 33: 50S ribosomal protein L5

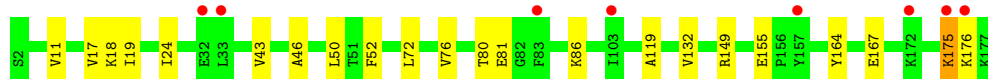
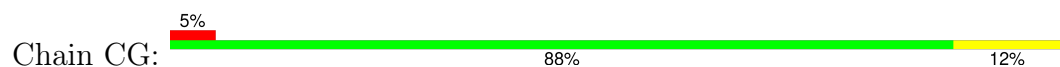


- Molecule 33: 50S ribosomal protein L5

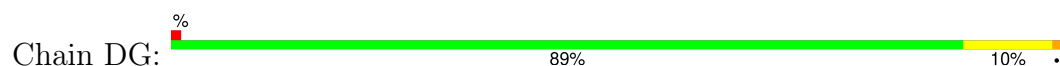




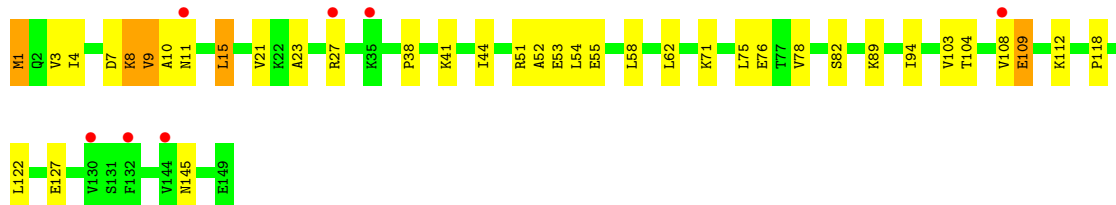
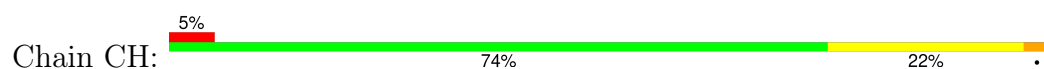
- Molecule 34: 50S ribosomal protein L6



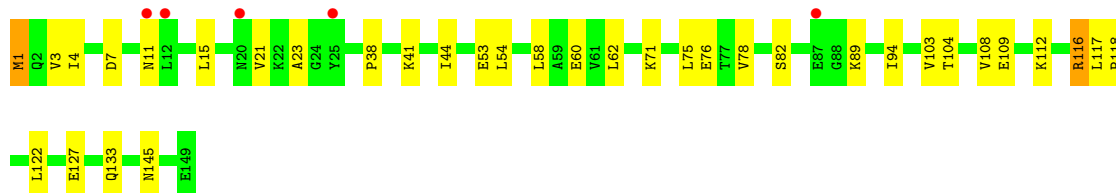
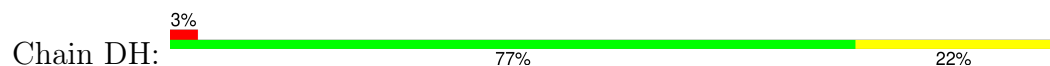
- Molecule 34: 50S ribosomal protein L6



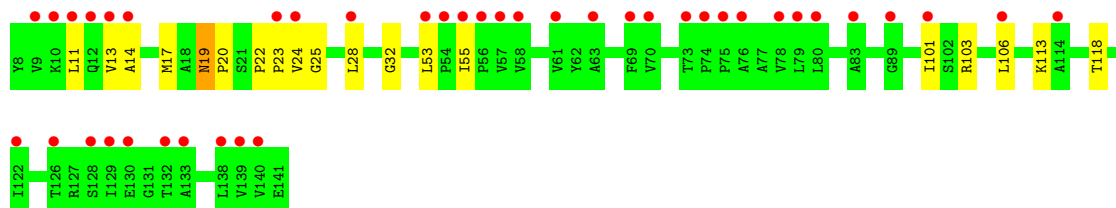
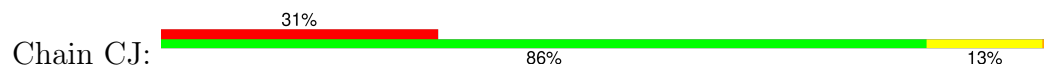
- Molecule 35: 50S ribosomal protein L9



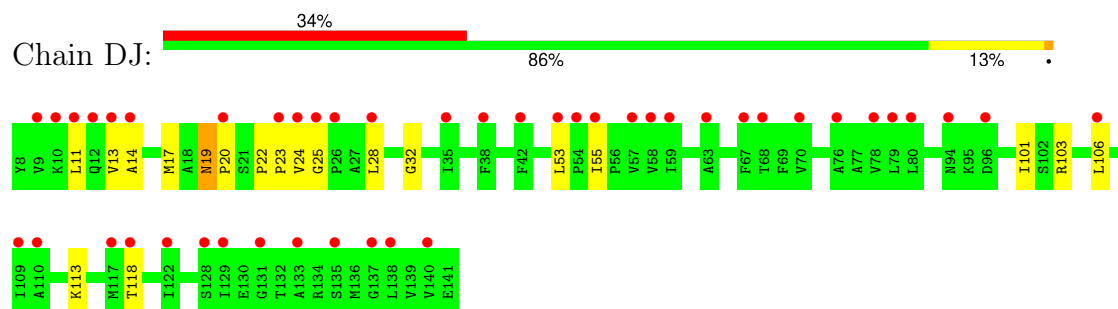
- Molecule 35: 50S ribosomal protein L9



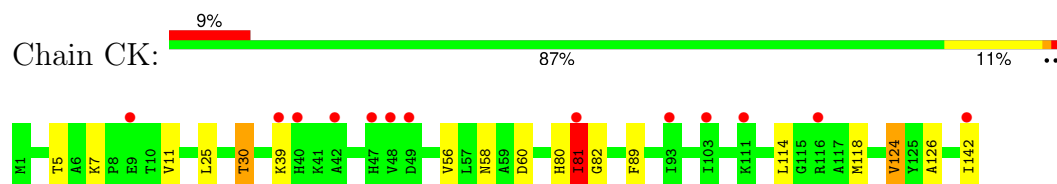
- Molecule 36: 50S ribosomal protein L11



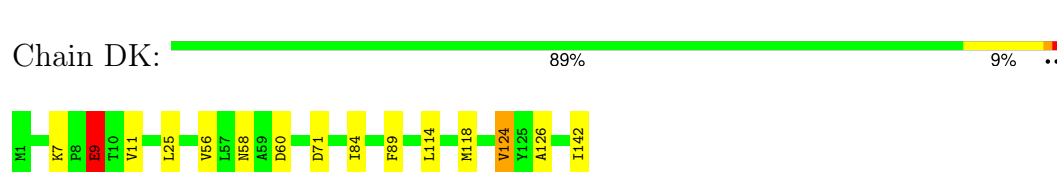
- Molecule 36: 50S ribosomal protein L11



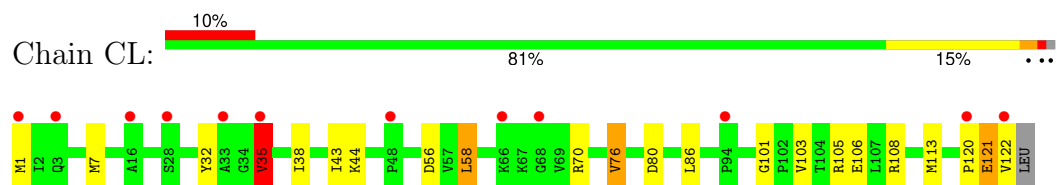
- Molecule 37: 50S ribosomal protein L13



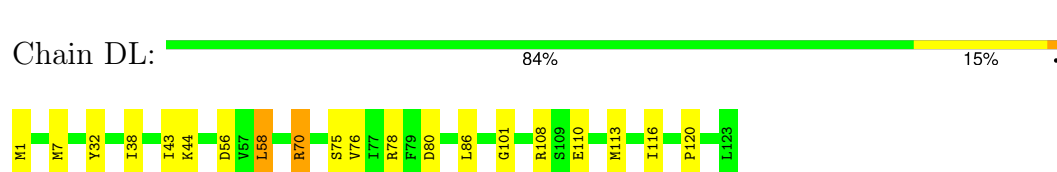
- Molecule 37: 50S ribosomal protein L13



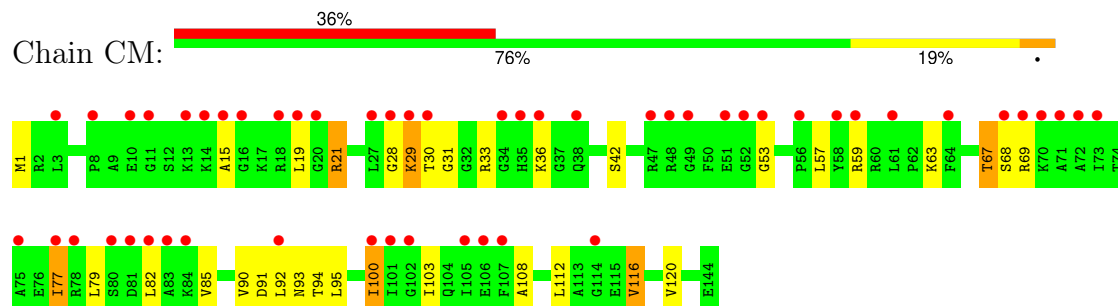
- Molecule 38: 50S ribosomal protein L14



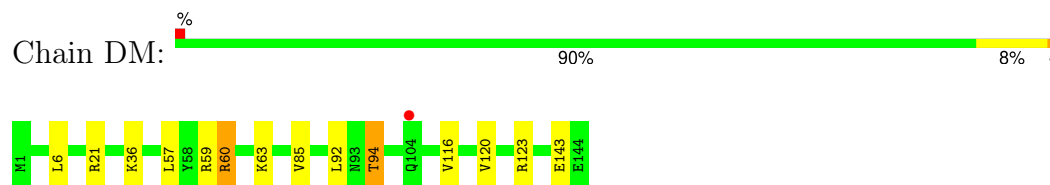
- Molecule 38: 50S ribosomal protein L14



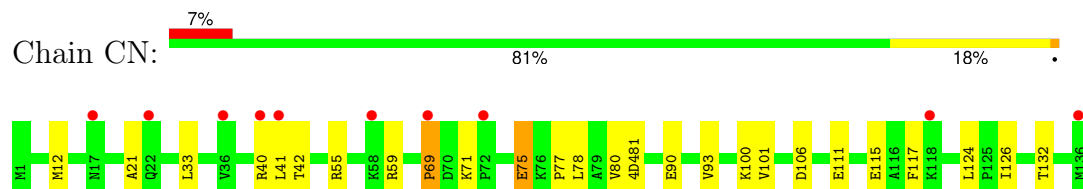
- Molecule 39: 50S ribosomal protein L15



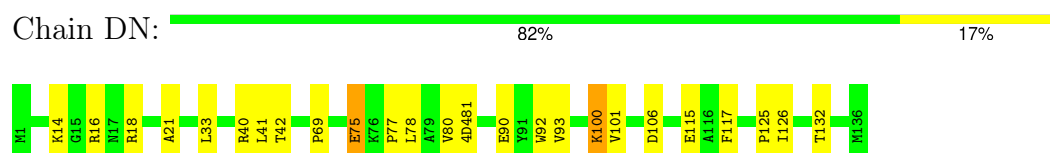
- Molecule 39: 50S ribosomal protein L15



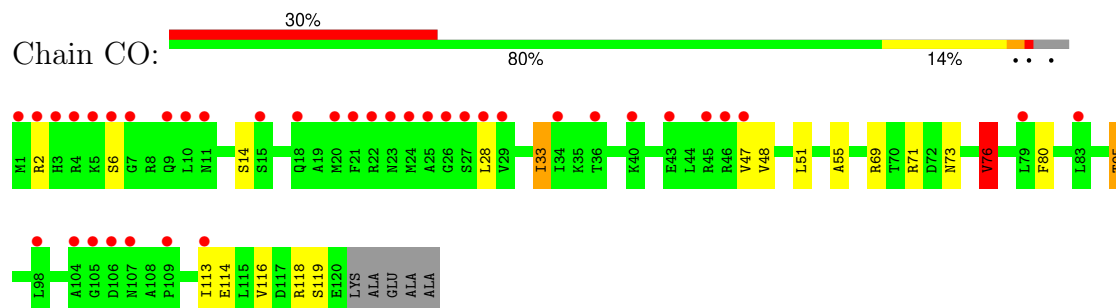
- Molecule 40: 50S ribosomal protein L16



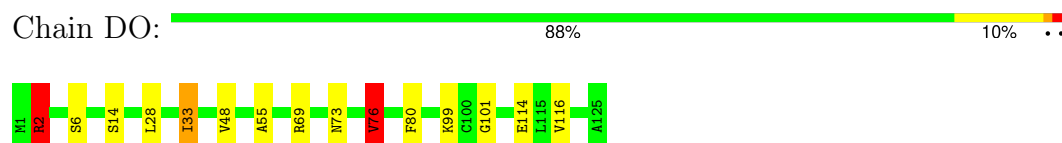
- Molecule 40: 50S ribosomal protein L16



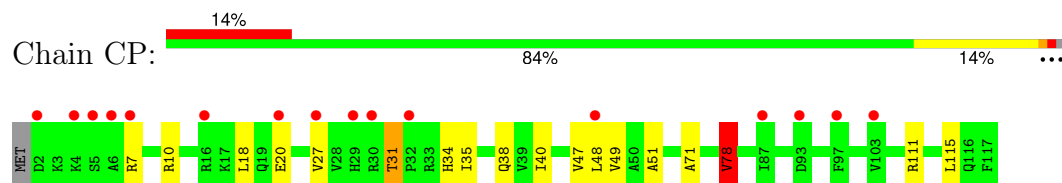
- Molecule 41: 50S ribosomal protein L17



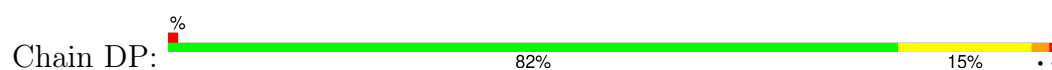
- Molecule 41: 50S ribosomal protein L17



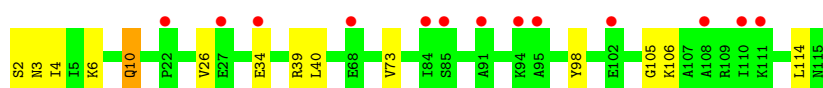
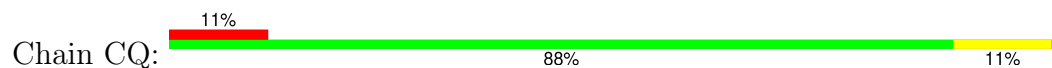
- Molecule 42: 50S ribosomal protein L18



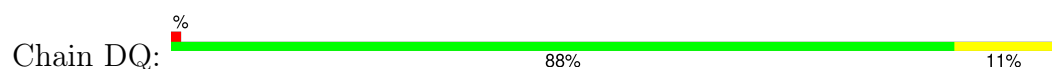
- Molecule 42: 50S ribosomal protein L18



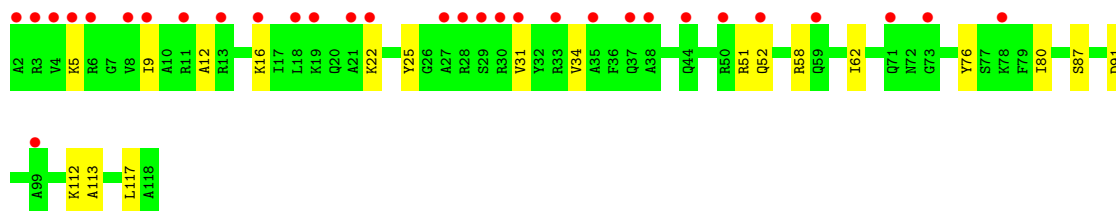
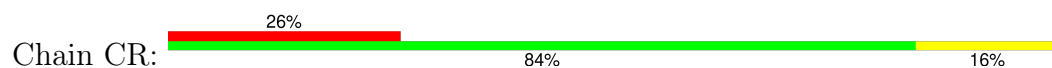
- Molecule 43: 50S ribosomal protein L19



- Molecule 43: 50S ribosomal protein L19



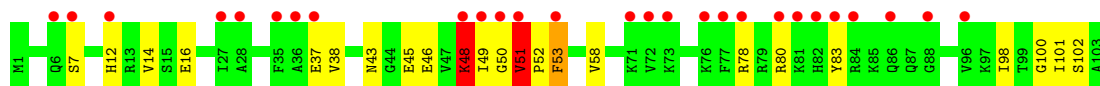
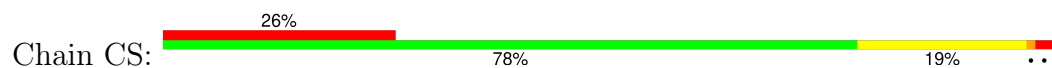
- Molecule 44: 50S ribosomal protein L20



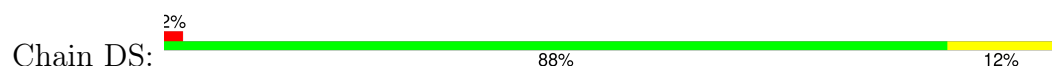
- Molecule 44: 50S ribosomal protein L20



- Molecule 45: 50S ribosomal protein L21

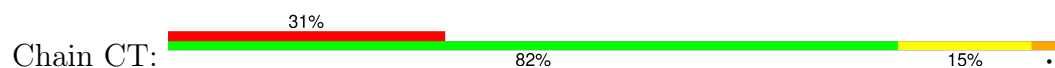


- Molecule 45: 50S ribosomal protein L21

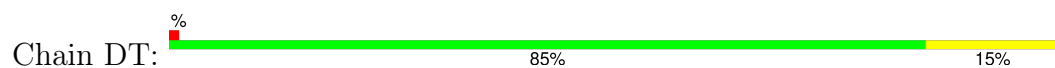




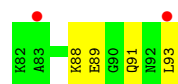
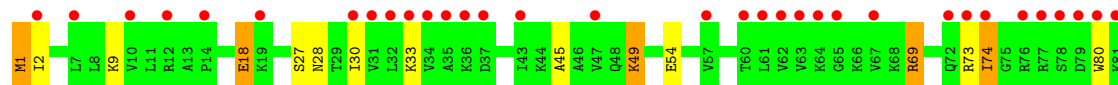
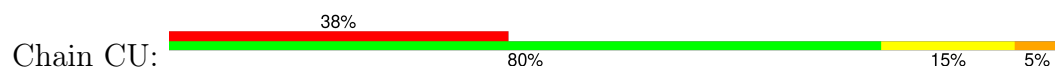
- Molecule 46: 50S ribosomal protein L22



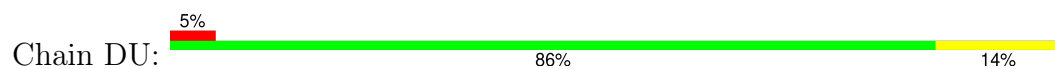
- Molecule 46: 50S ribosomal protein L22



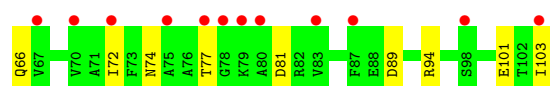
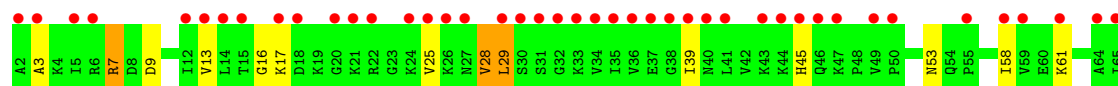
- Molecule 47: 50S ribosomal protein L23



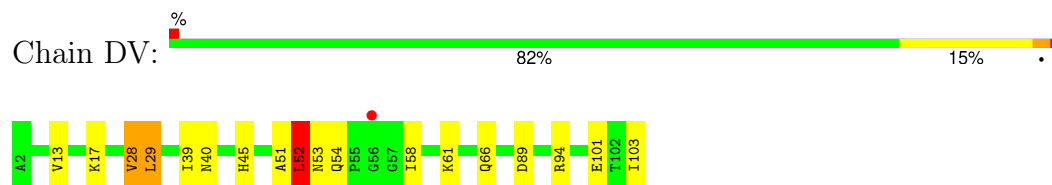
- Molecule 47: 50S ribosomal protein L23



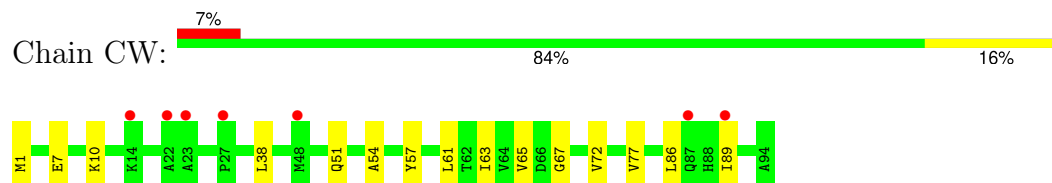
- Molecule 48: 50S ribosomal protein L24



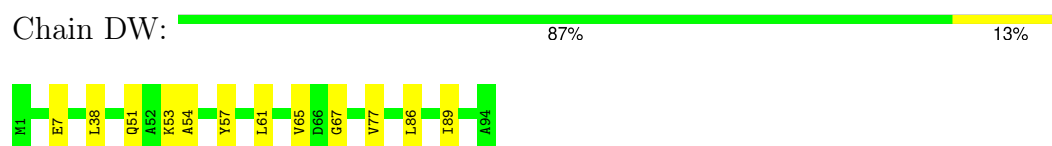
- Molecule 48: 50S ribosomal protein L24



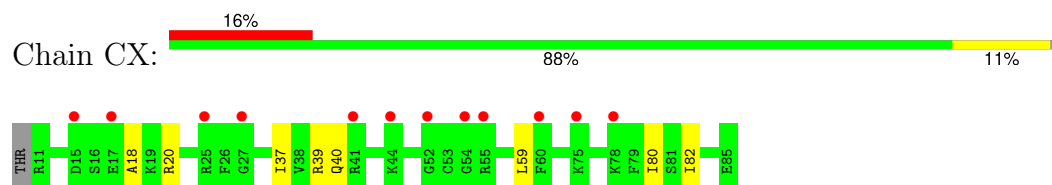
- Molecule 49: 50S ribosomal protein L25



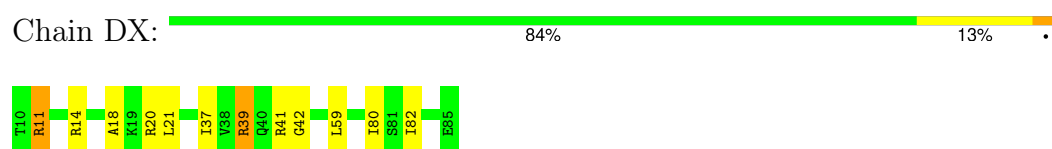
- Molecule 49: 50S ribosomal protein L25



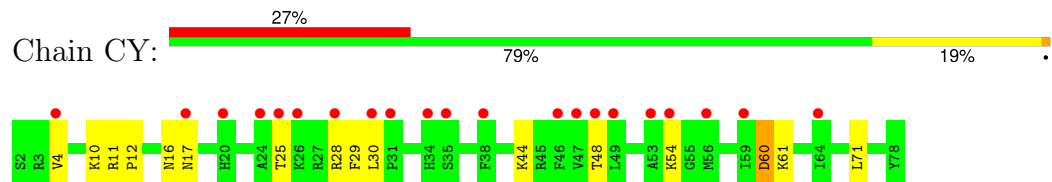
- Molecule 50: 50S ribosomal protein L27



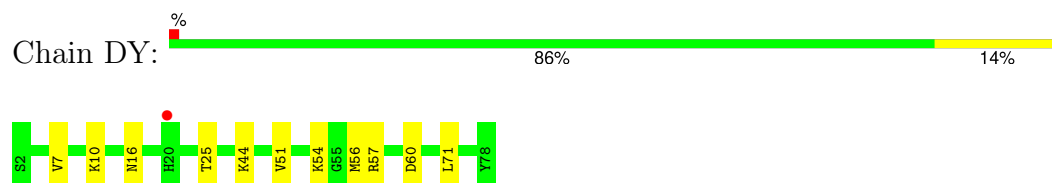
- Molecule 50: 50S ribosomal protein L27



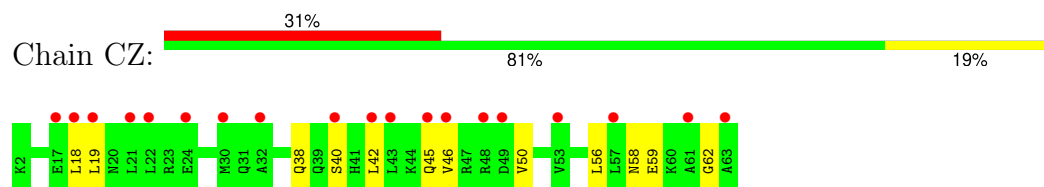
- Molecule 51: 50S ribosomal protein L28



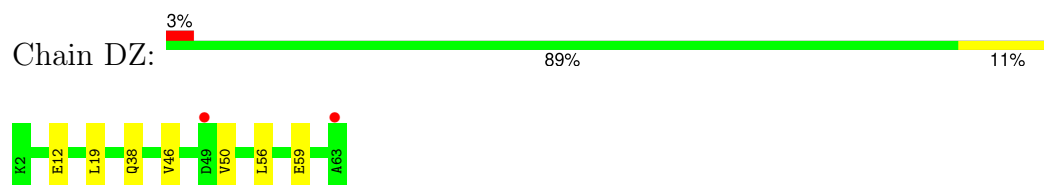
- Molecule 51: 50S ribosomal protein L28



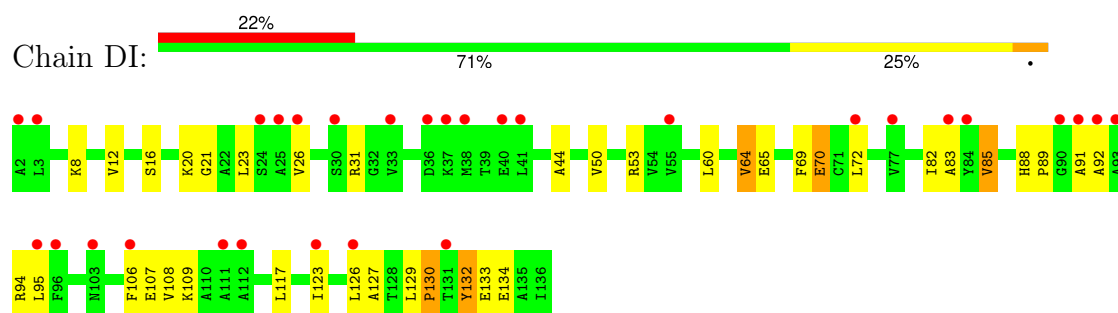
- Molecule 52: 50S ribosomal protein L29



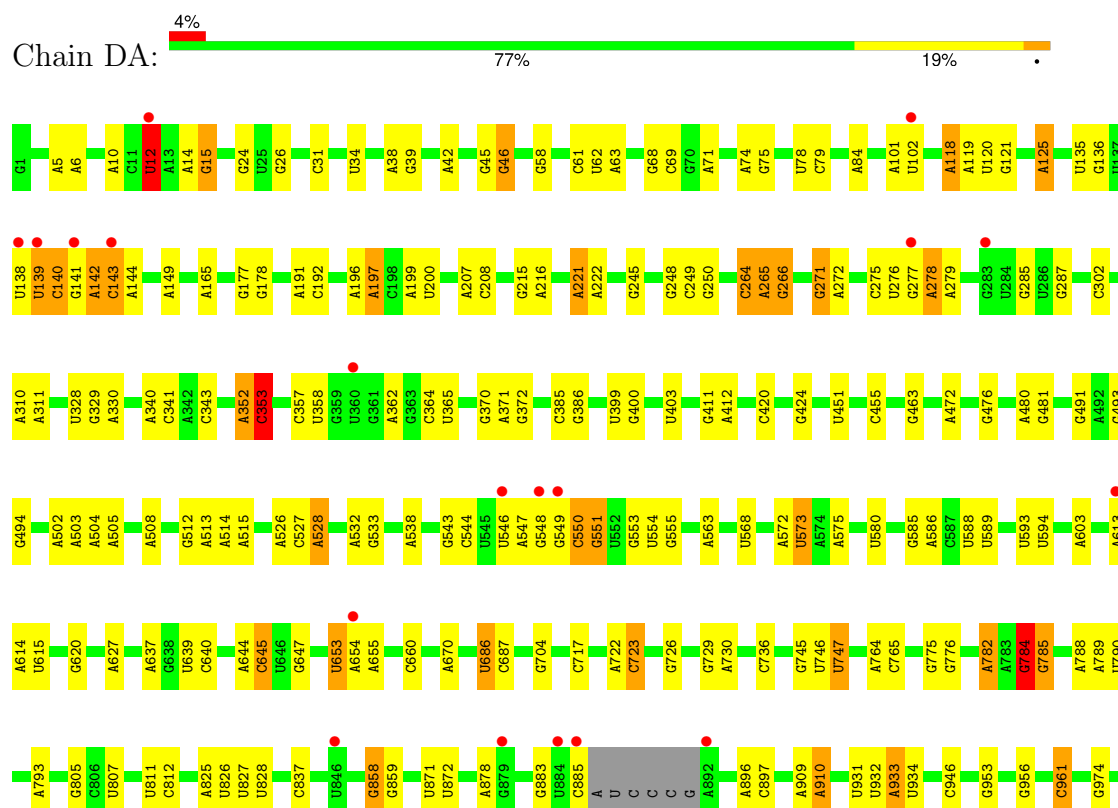
- Molecule 52: 50S ribosomal protein L29

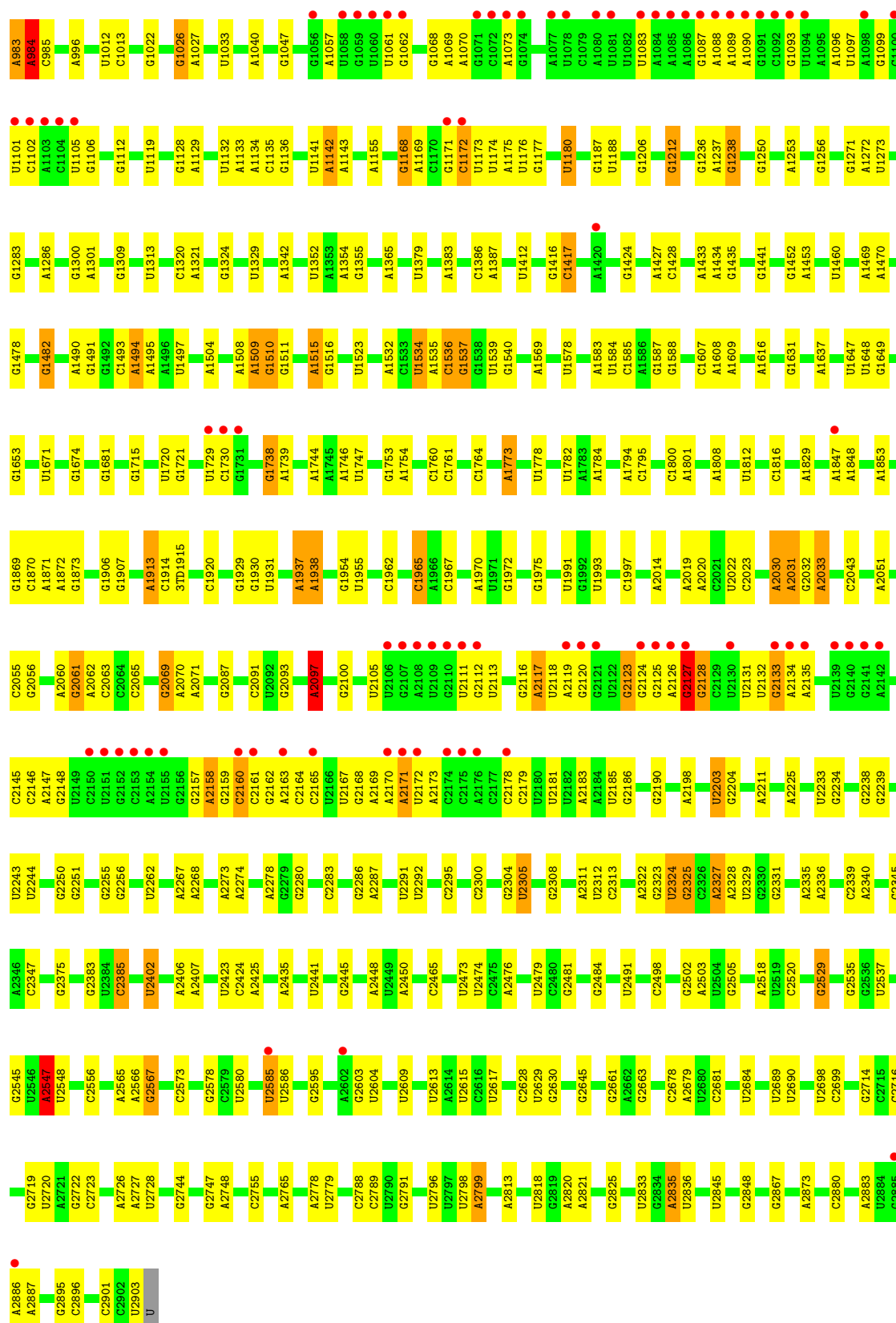


- Molecule 53: 50S ribosomal protein L10



- Molecule 54: 23S rRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 435.70Å 625.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.00 48.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-3.00) 99.1 (48.61-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.172 , 0.193 0.184 , 0.207	Depositor DCC
R_{free} test set	4504 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295261	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PUT, 4D4, EDO, PGE, GUN, 2MA, 1PE, PSU, MG, TAC, H2U, 2MG, UR3, PG4, ZN, D2T, 4OC, 3TD, OMC, MEQ, OMU, ACY, MA6, G7M, SPD, 5MC, TRS, 1MG, MPD, OMG, 6MZ, 5MU, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.70	10/36597 (0.0%)	0.69	1/57088 (0.0%)
1	BA	0.69	11/36572 (0.0%)	0.68	2/57049 (0.0%)
2	AB	0.81	0/1784	1.39	7/2403 (0.3%)
2	BB	0.81	0/1784	1.39	5/2403 (0.2%)
3	AC	0.82	0/1652	1.31	8/2225 (0.4%)
3	BC	0.83	0/1652	1.34	10/2225 (0.4%)
4	AD	0.76	0/1665	1.38	7/2227 (0.3%)
4	BD	0.76	0/1665	1.41	9/2227 (0.4%)
5	AE	0.82	0/1157	1.44	7/1557 (0.4%)
5	BE	0.88	0/1118	1.45	9/1504 (0.6%)
6	AF	0.82	0/881	1.35	4/1189 (0.3%)
6	BF	0.84	0/835	1.49	11/1128 (1.0%)
7	AG	0.82	0/1196	1.39	3/1602 (0.2%)
7	BG	0.83	0/1196	1.38	3/1602 (0.2%)
8	AH	0.76	0/989	1.35	3/1326 (0.2%)
8	BH	0.75	0/989	1.33	3/1326 (0.2%)
9	AI	0.80	0/1034	1.32	2/1375 (0.1%)
9	BI	0.80	0/1034	1.32	2/1375 (0.1%)
10	AJ	0.79	1/806 (0.1%)	1.26	5/1089 (0.5%)
10	BJ	0.90	1/797 (0.1%)	1.32	6/1077 (0.6%)
11	AK	0.77	0/893	1.20	2/1205 (0.2%)
11	BK	0.75	0/893	1.26	3/1205 (0.2%)
12	AL	0.78	0/960	1.26	6/1286 (0.5%)
12	BL	0.77	0/960	1.27	5/1286 (0.4%)
13	AM	0.92	1/893 (0.1%)	1.53	9/1193 (0.8%)
13	BM	0.91	0/893	1.52	14/1193 (1.2%)
14	AN	0.82	0/817	1.37	1/1088 (0.1%)
14	BN	0.79	0/817	1.35	1/1088 (0.1%)
15	AO	0.77	0/722	1.45	1/964 (0.1%)
15	BO	0.76	0/722	1.49	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.80	0/659	1.30	5/884 (0.6%)
16	BP	0.85	0/659	1.42	10/884 (1.1%)
17	AQ	0.82	0/658	1.24	4/881 (0.5%)
17	BQ	0.89	0/658	1.35	4/881 (0.5%)
18	AR	0.82	0/463	1.39	4/621 (0.6%)
18	BR	0.84	0/463	1.38	3/621 (0.5%)
19	AS	0.88	0/653	1.24	0/877
19	BS	0.88	0/653	1.25	0/877
20	AT	0.85	0/676	1.54	3/895 (0.3%)
20	BT	0.95	1/671 (0.1%)	1.63	5/888 (0.6%)
21	AU	0.70	0/472	1.36	2/627 (0.3%)
21	BU	0.69	0/472	1.39	2/627 (0.3%)
22	C1	0.86	0/450	1.28	0/599
22	D1	0.95	0/450	1.25	0/599
23	C2	0.88	1/416 (0.2%)	1.29	2/554 (0.4%)
23	D2	0.84	0/421	1.28	1/561 (0.2%)
24	C3	0.76	0/380	1.44	0/498
24	D3	0.88	0/380	1.48	1/498 (0.2%)
25	C4	0.77	0/513	1.23	0/676
25	D4	0.84	0/513	1.25	0/676
26	C5	0.74	0/303	1.24	2/397 (0.5%)
26	D5	0.87	1/303 (0.3%)	1.19	0/397
27	C0	0.87	0/453	1.37	0/605
27	D0	0.97	0/467	1.32	1/623 (0.2%)
28	CB	0.63	0/2828	0.68	1/4410 (0.0%)
28	DB	0.72	0/2872	0.71	0/4478
29	CC	0.76	0/2122	1.29	11/2852 (0.4%)
29	DC	0.79	0/2122	1.28	7/2852 (0.2%)
30	CD	0.76	0/1576	1.17	1/2119 (0.0%)
30	DD	0.84	0/1576	1.15	1/2119 (0.0%)
31	CA	0.72	46/69143 (0.1%)	0.69	8/107862 (0.0%)
32	CE	0.78	0/1571	1.34	8/2113 (0.4%)
32	DE	0.82	0/1571	1.30	4/2113 (0.2%)
33	CF	0.77	0/1435	1.39	13/1926 (0.7%)
33	DF	0.81	0/1435	1.38	10/1926 (0.5%)
34	CG	0.75	0/1343	1.26	4/1816 (0.2%)
34	DG	0.77	0/1343	1.22	4/1816 (0.2%)
35	CH	0.86	0/1121	1.32	4/1515 (0.3%)
35	DH	0.86	0/1121	1.31	0/1515
36	CJ	0.95	0/993	1.36	3/1341 (0.2%)
36	DJ	0.94	0/993	1.36	3/1341 (0.2%)
37	CK	0.72	0/1152	1.30	5/1551 (0.3%)
37	DK	0.88	0/1152	1.31	5/1551 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CL	0.81	0/947	1.21	2/1268 (0.2%)
38	DL	0.85	0/955	1.21	0/1279
39	CM	0.82	1/1062 (0.1%)	1.36	8/1413 (0.6%)
39	DM	0.79	0/1062	1.26	0/1413
40	CN	0.78	0/1081	1.26	4/1443 (0.3%)
40	DN	0.86	0/1092	1.27	2/1457 (0.1%)
41	CO	0.79	0/973	1.28	1/1301 (0.1%)
41	DO	0.91	0/1006	1.35	6/1345 (0.4%)
42	CP	0.76	0/902	1.42	1/1209 (0.1%)
42	DP	0.84	0/910	1.40	3/1219 (0.2%)
43	CQ	0.71	0/929	1.16	2/1242 (0.2%)
43	DQ	0.76	0/929	1.17	2/1242 (0.2%)
44	CR	0.73	0/960	1.36	4/1278 (0.3%)
44	DR	0.87	0/960	1.33	1/1278 (0.1%)
45	CS	0.77	0/829	1.20	3/1107 (0.3%)
45	DS	0.86	0/829	1.20	1/1107 (0.1%)
46	CT	0.74	0/864	1.29	2/1156 (0.2%)
46	DT	0.88	0/864	1.25	1/1156 (0.1%)
47	CU	0.80	0/745	1.30	2/994 (0.2%)
47	DU	0.84	0/745	1.32	2/994 (0.2%)
48	CV	0.81	0/788	1.36	8/1051 (0.8%)
48	DV	0.83	0/788	1.31	8/1051 (0.8%)
49	CW	0.73	0/766	1.24	4/1025 (0.4%)
49	DW	0.83	0/766	1.26	4/1025 (0.4%)
50	CX	0.71	0/576	1.17	0/762
50	DX	0.88	0/598	1.24	3/790 (0.4%)
51	CY	0.70	0/635	1.33	3/848 (0.4%)
51	DY	0.75	0/635	1.31	2/848 (0.2%)
52	CZ	0.74	0/502	1.47	0/667
52	DZ	0.77	0/502	1.46	0/667
53	DI	0.92	0/1037	1.51	6/1402 (0.4%)
54	DA	0.80	32/69364 (0.0%)	0.75	2/108207 (0.0%)
All	All	0.76	106/309249 (0.0%)	0.92	377/462175 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	8
40	CN	0	1
40	DN	0	1
54	DA	0	41
All	All	0	56

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.61	1.28	1.42
54	DA	12	U	C1'-N1	8.96	1.61	1.48
54	DA	2097	A	O5'-C5'	-8.65	1.29	1.42
31	CA	769	U	C1'-N1	8.12	1.60	1.48
54	DA	1237	A	C3'-O3'	-8.09	1.31	1.43
31	CA	12	U	C1'-N1	8.03	1.60	1.48
31	CA	1777	U	C1'-N1	7.42	1.59	1.48
31	CA	2069	G7M	O3'-P	7.15	1.63	1.56
31	CA	2425	A	C3'-O3'	7.08	1.53	1.43
54	DA	2585	U	C1'-N1	6.97	1.57	1.47
1	BA	5	U	C1'-N1	6.94	1.58	1.48
31	CA	2233	U	C1'-N1	6.92	1.58	1.48
54	DA	2069	G7M	O3'-P	6.82	1.63	1.56
1	AA	5	U	C1'-N1	6.79	1.58	1.48
31	CA	2225	A	C3'-O3'	6.63	1.53	1.43
31	CA	1658	C	C1'-N1	6.60	1.58	1.48
31	CA	692	C	C1'-N1	6.55	1.58	1.48
54	DA	2585	U	C3'-O3'	6.37	1.52	1.43
31	CA	946	C	C1'-N1	6.35	1.57	1.48
1	AA	1354	U	C1'-N1	6.32	1.57	1.48
31	CA	1825	U	C1'-N1	6.27	1.57	1.48
31	CA	1379	U	C3'-O3'	6.17	1.51	1.42
31	CA	451	U	C1'-N1	6.16	1.57	1.48
1	AA	956	U	C1'-N1	6.09	1.57	1.48
31	CA	2017	U	C1'-N1	6.09	1.57	1.48
31	CA	546	U	C1'-N1	6.08	1.57	1.48
54	DA	2547	A	O5'-C5'	-5.95	1.33	1.42
31	CA	1790	C	C1'-N1	5.95	1.57	1.48
1	BA	1008	U	O5'-C5'	-5.94	1.33	1.42
54	DA	653	U	C1'-N1	5.92	1.57	1.48
1	BA	1493	A	C3'-O3'	5.92	1.51	1.42
31	CA	20	C	C1'-N1	5.90	1.57	1.48
31	CA	1314	C	C1'-N1	5.83	1.57	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1313	U	C1'-N1	5.81	1.57	1.48
1	AA	632	U	C1'-N1	5.79	1.57	1.48
31	CA	653	U	C1'-N1	5.78	1.57	1.48
31	CA	995	C	O5'-C5'	-5.77	1.34	1.42
54	DA	140	C	C1'-N1	5.75	1.56	1.47
31	CA	2779	U	C1'-N1	5.71	1.56	1.47
1	AA	955	U	C1'-N1	5.71	1.57	1.48
31	CA	691	C	C1'-N1	5.71	1.57	1.48
1	BA	209	U	C1'-N1	5.70	1.57	1.48
31	CA	817	C	C1'-N1	5.69	1.56	1.48
31	CA	2456	C	C1'-N1	5.67	1.56	1.48
54	DA	1965	C	C3'-O3'	-5.64	1.33	1.42
26	D5	26	ILE	CG1-CD1	5.64	1.73	1.51
31	CA	1376	C	C1'-N1	5.61	1.56	1.48
39	CM	77	ILE	CG1-CD1	-5.59	1.29	1.51
1	BA	956	U	C1'-N1	5.58	1.56	1.48
1	BA	1354	U	C1'-N1	5.58	1.56	1.48
1	BA	955	U	C1'-N1	5.57	1.56	1.48
10	AJ	57	VAL	CA-C	5.57	1.59	1.52
31	CA	2354	C	C1'-N1	5.56	1.56	1.48
23	C2	5	ILE	CA-C	5.50	1.59	1.52
54	DA	1441	G	O5'-C5'	-5.50	1.34	1.42
1	BA	221	C	C1'-N1	5.50	1.56	1.48
54	DA	2402	U	C1'-N1	5.49	1.56	1.48
31	CA	1788	C	C1'-N1	5.47	1.56	1.48
31	CA	790	U	C1'-N1	5.46	1.56	1.48
31	CA	1352	U	C1'-N1	5.43	1.56	1.48
31	CA	1994	C	C1'-N1	5.43	1.56	1.48
10	BJ	57	VAL	CA-C	5.42	1.59	1.52
1	AA	221	C	C1'-N1	5.40	1.56	1.48
1	AA	485	U	C1'-N1	5.40	1.55	1.47
54	DA	12	U	O5'-C5'	5.39	1.50	1.42
13	AM	114	LYS	CA-C	5.37	1.58	1.53
54	DA	1188	U	C3'-O3'	-5.35	1.34	1.42
54	DA	1920	C	C1'-N1	5.35	1.56	1.48
31	CA	1306	C	C1'-N1	5.34	1.56	1.48
1	AA	845	A	O5'-C5'	5.34	1.50	1.42
54	DA	1534	U	C1'-N1	5.33	1.56	1.48
54	DA	275	C	C1'-N1	5.29	1.56	1.48
31	CA	1971	U	C1'-N1	5.27	1.56	1.48
54	DA	1412	U	C1'-N1	5.27	1.56	1.48
54	DA	2127	G	C3'-O3'	5.27	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1584	U	C1'-N1	5.26	1.56	1.48
31	CA	678	C	C1'-N1	5.26	1.56	1.48
54	DA	139	U	C1'-N1	5.24	1.55	1.47
31	CA	2215	C	C1'-N1	5.22	1.56	1.48
54	DA	961	C	C1'-N1	5.22	1.55	1.47
54	DA	353	C	C1'-N1	5.22	1.56	1.48
31	CA	2465	C	C1'-N1	5.19	1.56	1.48
54	DA	2617	U	O5'-C5'	-5.16	1.34	1.42
31	CA	2232	C	C1'-N1	5.16	1.56	1.48
54	DA	2203	U	C1'-N1	5.16	1.56	1.48
31	CA	2585	U	C1'-N1	5.15	1.56	1.48
1	BA	632	U	C1'-N1	5.15	1.56	1.48
54	DA	1174	U	C1'-N1	5.14	1.56	1.48
31	CA	1412	U	C1'-N1	5.14	1.56	1.48
31	CA	961	C	C1'-N1	5.11	1.55	1.47
1	AA	1298	U	C1'-N1	5.09	1.55	1.47
31	CA	140	C	C1'-N1	5.08	1.55	1.47
31	CA	114	U	C1'-N1	5.08	1.56	1.48
1	AA	272	C	C1'-N1	5.08	1.56	1.48
1	BA	1498	UR3	O3'-P	5.07	1.61	1.56
54	DA	784	G	C3'-O3'	5.07	1.49	1.42
54	DA	736	C	C3'-O3'	-5.06	1.34	1.42
31	CA	557	C	C1'-N1	5.04	1.56	1.48
54	DA	2061	G	O5'-C5'	-5.04	1.35	1.42
54	DA	2901	C	C1'-N1	5.04	1.56	1.48
31	CA	353	C	C1'-N1	5.04	1.56	1.48
31	CA	2861	U	C1'-N1	5.03	1.55	1.48
1	BA	527	G7M	O3'-P	5.02	1.61	1.56
54	DA	2300	C	C1'-N1	5.01	1.55	1.48
20	BT	5	LYS	CA-C	5.00	1.59	1.52
31	CA	2006	C	C1'-N1	5.00	1.55	1.48

All (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DI	132	TYR	CA-C-N	9.82	139.38	121.70
53	DI	132	TYR	C-N-CA	9.82	139.38	121.70
5	BE	50	TYR	CA-C-O	-9.01	113.28	119.68
33	DF	10	ASP	CA-CB-CG	9.00	121.60	112.60
6	BF	90	MET	CA-C-N	8.72	133.64	120.82
6	BF	90	MET	C-N-CA	8.72	133.64	120.82
27	D0	10	THR	N-CA-CB	-8.34	99.81	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DC	260	ASN	CA-C-N	8.16	131.56	120.38
29	DC	260	ASN	C-N-CA	8.16	131.56	120.38
53	DI	106	PHE	CA-CB-CG	8.01	121.81	113.80
6	AF	55	HIS	N-CA-C	-7.61	97.00	109.40
23	D2	5	ILE	N-CA-C	-7.49	105.25	112.29
6	BF	55	HIS	N-CA-C	-7.45	97.25	109.40
42	DP	78	VAL	N-CA-CB	7.30	119.09	110.55
33	CF	107	ALA	CA-C-N	7.27	124.82	120.24
33	CF	107	ALA	C-N-CA	7.27	124.82	120.24
6	BF	79	ARG	CA-C-N	7.23	129.84	120.44
6	BF	79	ARG	C-N-CA	7.23	129.84	120.44
2	BB	126	PHE	CA-CB-CG	7.16	120.95	113.80
39	CM	68	SER	CA-C-N	7.12	135.13	121.54
39	CM	68	SER	C-N-CA	7.12	135.13	121.54
29	DC	156	ARG	CB-CG-CD	-7.10	94.96	111.30
16	BP	42	ILE	CA-C-N	7.09	130.11	120.54
16	BP	42	ILE	C-N-CA	7.09	130.11	120.54
42	CP	78	VAL	N-CA-CB	7.06	118.81	110.55
10	AJ	76	ILE	CA-C-N	7.03	129.56	120.56
10	AJ	76	ILE	C-N-CA	7.03	129.56	120.56
20	BT	6	SER	N-CA-C	-7.01	104.54	113.23
6	BF	91	ARG	N-CA-C	7.01	119.35	110.24
2	AB	126	PHE	CA-CB-CG	6.99	120.79	113.80
20	BT	43	ASP	CA-CB-CG	6.97	119.57	112.60
8	BH	109	GLY	N-CA-C	6.93	119.11	112.04
20	BT	6	SER	CA-C-N	6.88	130.19	120.28
20	BT	6	SER	C-N-CA	6.88	130.19	120.28
44	CR	12	ALA	CA-C-N	6.86	129.80	120.54
44	CR	12	ALA	C-N-CA	6.86	129.80	120.54
35	CH	8	LYS	CA-C-N	6.84	134.28	121.97
35	CH	8	LYS	C-N-CA	6.84	134.28	121.97
5	AE	50	TYR	CA-C-N	-6.79	117.37	122.33
5	AE	50	TYR	C-N-CA	-6.79	117.37	122.33
13	AM	96	PRO	CA-C-N	6.78	129.24	120.56
13	AM	96	PRO	C-N-CA	6.78	129.24	120.56
5	AE	55	GLU	CA-C-N	6.77	126.93	120.43
5	AE	55	GLU	C-N-CA	6.77	126.93	120.43
8	AH	109	GLY	N-CA-C	6.74	118.92	112.04
13	BM	96	PRO	CA-C-N	6.71	129.14	120.56
13	BM	96	PRO	C-N-CA	6.71	129.14	120.56
11	BK	71	ALA	N-CA-C	-6.67	103.49	111.69
32	CE	7	ASP	CA-CB-CG	6.61	119.21	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	CF	46	ASP	CA-CB-CG	6.59	119.19	112.60
29	DC	264	ASP	CA-CB-CG	6.55	119.15	112.60
5	BE	55	GLU	CA-C-N	6.54	126.70	120.43
5	BE	55	GLU	C-N-CA	6.54	126.70	120.43
33	CF	134	GLU	CB-CG-CD	6.52	123.69	112.60
34	CG	175	LYS	CA-C-N	6.50	133.96	121.54
34	CG	175	LYS	C-N-CA	6.50	133.96	121.54
3	BC	61	ALA	CA-C-N	6.50	131.35	122.19
3	BC	61	ALA	C-N-CA	6.50	131.35	122.19
33	CF	21	ASN	CA-CB-CG	6.46	119.06	112.60
40	CN	106	ASP	CA-CB-CG	6.41	119.01	112.60
4	AD	99	ASP	CA-CB-CG	6.40	119.00	112.60
46	DT	65	ASP	CA-CB-CG	6.39	119.00	112.60
33	DF	46	ASP	CA-CB-CG	6.38	118.98	112.60
10	BJ	37	ARG	CA-C-N	6.35	131.84	121.87
10	BJ	37	ARG	C-N-CA	6.35	131.84	121.87
54	DA	271	G	C2'-C3'-O3'	6.35	119.02	109.50
37	DK	9	GLU	CB-CG-CD	6.32	123.35	112.60
39	CM	68	SER	N-CA-C	6.32	118.73	111.02
3	BC	178	LEU	CA-C-N	6.32	129.38	120.28
3	BC	178	LEU	C-N-CA	6.32	129.38	120.28
4	BD	99	ASP	CA-CB-CG	6.30	118.90	112.60
40	DN	106	ASP	CA-CB-CG	6.29	118.89	112.60
29	CC	239	ASN	CA-CB-CG	6.27	118.87	112.60
16	AP	23	ASP	CA-CB-CG	6.27	118.87	112.60
24	D3	44	VAL	N-CA-CB	6.26	118.13	111.00
6	AF	79	ARG	CA-C-N	6.25	128.57	120.44
6	AF	79	ARG	C-N-CA	6.25	128.57	120.44
53	DI	20	LYS	CA-C-N	6.24	127.05	119.99
53	DI	20	LYS	C-N-CA	6.24	127.05	119.99
37	CK	80	HIS	CA-C-N	6.22	133.18	121.97
37	CK	80	HIS	C-N-CA	6.22	133.18	121.97
48	CV	9	ASP	CA-CB-CG	6.19	118.79	112.60
16	BP	23	ASP	CA-CB-CG	6.13	118.73	112.60
33	DF	123	ASP	CA-CB-CG	6.13	118.73	112.60
48	DV	53	ASN	CA-C-N	6.12	128.97	120.65
48	DV	53	ASN	C-N-CA	6.12	128.97	120.65
37	CK	60	ASP	CA-CB-CG	6.11	118.71	112.60
13	AM	54	ASP	CA-CB-CG	6.10	118.70	112.60
13	BM	11	ASP	CA-C-N	6.07	131.19	122.40
13	BM	11	ASP	C-N-CA	6.07	131.19	122.40
20	BT	84	ASN	CA-CB-CG	6.02	118.62	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	DE	64	GLY	N-CA-C	6.00	122.22	115.08
3	AC	178	LEU	CA-C-N	6.00	128.92	120.28
3	AC	178	LEU	C-N-CA	6.00	128.92	120.28
11	BK	118	HIS	CA-C-N	5.99	132.98	121.54
11	BK	118	HIS	C-N-CA	5.99	132.98	121.54
29	DC	70	ASN	CA-CB-CG	5.97	118.57	112.60
16	AP	47	GLU	CA-C-N	5.95	132.91	121.54
16	AP	47	GLU	C-N-CA	5.95	132.91	121.54
18	BR	34	THR	CA-C-N	5.95	128.18	120.44
18	BR	34	THR	C-N-CA	5.95	128.18	120.44
37	DK	60	ASP	CA-CB-CG	5.94	118.54	112.60
20	AT	58	VAL	N-CA-CB	5.91	118.13	110.57
5	AE	106	ILE	CB-CA-C	5.88	118.41	111.59
36	CJ	22	PRO	N-CA-C	5.87	117.86	110.70
29	CC	157	SER	CA-C-N	5.87	132.74	121.54
29	CC	157	SER	C-N-CA	5.87	132.74	121.54
6	AF	80	PHE	CA-CB-CG	5.85	119.65	113.80
36	DJ	22	PRO	N-CA-C	5.85	117.84	110.70
41	DO	99	LYS	CA-C-N	-5.85	116.87	123.13
41	DO	99	LYS	C-N-CA	-5.85	116.87	123.13
45	CS	50	GLY	CA-C-N	5.85	131.24	122.17
45	CS	50	GLY	C-N-CA	5.85	131.24	122.17
39	CM	91	ASP	CA-CB-CG	5.80	118.40	112.60
39	CM	15	ALA	N-CA-C	5.79	118.06	111.11
14	BN	84	VAL	N-CA-C	-5.78	105.10	110.53
6	BF	98	GLU	CA-C-N	5.77	132.56	121.54
6	BF	98	GLU	C-N-CA	5.77	132.56	121.54
18	AR	34	THR	CA-C-N	5.77	128.01	120.28
18	AR	34	THR	C-N-CA	5.77	128.01	120.28
29	CC	208	ALA	CA-C-N	5.76	126.37	119.98
29	CC	208	ALA	C-N-CA	5.76	126.37	119.98
48	CV	3	ALA	CA-C-N	5.73	132.49	121.54
48	CV	3	ALA	C-N-CA	5.73	132.49	121.54
48	DV	28	VAL	N-CA-CB	5.73	119.08	111.64
12	BL	42	PRO	CA-C-N	5.72	129.23	120.82
12	BL	42	PRO	C-N-CA	5.72	129.23	120.82
1	BA	1362	A	C1'-O4'-C4'	-5.70	104.00	109.70
8	AH	33	LYS	CA-C-N	5.68	127.72	120.56
8	AH	33	LYS	C-N-CA	5.68	127.72	120.56
4	AD	39	GLY	CA-C-N	5.67	127.82	120.44
4	AD	39	GLY	C-N-CA	5.67	127.82	120.44
9	BI	99	ARG	CA-C-N	5.66	128.14	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BI	99	ARG	C-N-CA	5.66	128.14	120.38
16	BP	19	VAL	N-CA-CB	5.64	117.43	111.00
33	DF	146	VAL	N-CA-CB	5.63	117.25	110.95
31	CA	271	G	C2'-C3'-O3'	5.62	117.93	109.50
3	BC	26	THR	CA-C-N	5.61	127.73	120.44
3	BC	26	THR	C-N-CA	5.61	127.73	120.44
4	BD	131	ASN	CA-CB-CG	5.61	118.21	112.60
12	BL	64	THR	CB-CA-C	5.60	118.99	109.75
2	AB	93	ASN	CA-CB-CG	5.59	118.19	112.60
48	CV	53	ASN	CA-C-N	5.58	127.07	120.09
48	CV	53	ASN	C-N-CA	5.58	127.07	120.09
14	AN	84	VAL	N-CA-C	-5.58	105.29	110.53
6	BF	80	PHE	CA-CB-CG	5.58	119.38	113.80
39	CM	67	THR	CA-C-N	5.57	128.54	120.79
39	CM	67	THR	C-N-CA	5.57	128.54	120.79
2	BB	93	ASN	CA-CB-CG	5.57	118.17	112.60
51	DY	60	ASP	CA-CB-CG	5.57	118.17	112.60
33	DF	13	VAL	CA-C-N	5.54	128.03	120.54
33	DF	13	VAL	C-N-CA	5.54	128.03	120.54
31	CA	974	G	N9-C1'-C2'	5.54	122.31	114.00
33	CF	13	VAL	CA-C-N	5.54	128.01	120.54
33	CF	13	VAL	C-N-CA	5.54	128.01	120.54
47	DU	92	ASN	CA-C-N	5.53	131.65	121.70
47	DU	92	ASN	C-N-CA	5.53	131.65	121.70
2	BB	204	ASP	CA-CB-CG	5.53	118.13	112.60
38	CL	121	GLU	CA-C-N	5.52	131.64	121.70
38	CL	121	GLU	C-N-CA	5.52	131.64	121.70
17	BQ	57	ASP	CA-CB-CG	5.52	118.12	112.60
13	AM	91	HIS	CA-C-N	5.51	130.05	120.68
13	AM	91	HIS	C-N-CA	5.51	130.05	120.68
32	CE	171	ASP	CA-CB-CG	5.51	118.11	112.60
17	BQ	51	ASN	CA-CB-CG	5.51	118.11	112.60
33	CF	164	GLU	CA-C-N	5.50	128.21	120.28
33	CF	164	GLU	C-N-CA	5.50	128.21	120.28
5	BE	105	ILE	N-CA-CB	5.50	120.31	111.23
44	CR	91	ASP	CA-CB-CG	5.50	118.10	112.60
9	AI	99	ARG	CA-C-N	5.49	127.90	120.38
9	AI	99	ARG	C-N-CA	5.49	127.90	120.38
32	CE	83	VAL	CA-C-N	5.49	127.90	120.44
32	CE	83	VAL	C-N-CA	5.49	127.90	120.44
43	DQ	3	ASN	CA-C-N	5.48	127.46	120.56
43	DQ	3	ASN	C-N-CA	5.48	127.46	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	CK	89	PHE	CA-C-N	5.46	127.92	120.54
37	CK	89	PHE	C-N-CA	5.46	127.92	120.54
17	AQ	57	ASP	CA-CB-CG	5.46	118.06	112.60
6	BF	92	THR	CA-C-N	5.46	131.12	122.61
6	BF	92	THR	C-N-CA	5.46	131.12	122.61
48	DV	51	ALA	CA-C-N	5.45	131.96	121.54
48	DV	51	ALA	C-N-CA	5.45	131.96	121.54
13	AM	14	HIS	CA-C-N	5.43	128.97	120.82
13	AM	14	HIS	C-N-CA	5.43	128.97	120.82
12	AL	38	TYR	N-CA-C	5.42	115.28	108.45
41	CO	76	VAL	N-CA-CB	5.42	118.72	110.58
36	CJ	118	THR	CA-C-N	5.42	125.25	120.10
36	CJ	118	THR	C-N-CA	5.42	125.25	120.10
13	BM	14	HIS	CA-C-N	5.41	128.93	120.82
13	BM	14	HIS	C-N-CA	5.41	128.93	120.82
33	CF	146	VAL	N-CA-CB	5.41	117.01	110.95
36	DJ	118	THR	CA-C-N	5.41	125.24	120.10
36	DJ	118	THR	C-N-CA	5.41	125.24	120.10
11	AK	118	HIS	CA-C-N	5.38	131.82	121.54
11	AK	118	HIS	C-N-CA	5.38	131.82	121.54
7	AG	151	PHE	CA-CB-CG	5.38	119.18	113.80
41	DO	76	VAL	N-CA-CB	5.38	118.64	110.58
12	AL	64	THR	CB-CA-C	5.37	118.61	109.75
33	DF	59	ALA	CA-C-N	5.37	127.32	120.56
33	DF	59	ALA	C-N-CA	5.37	127.32	120.56
10	BJ	58	ASN	CA-C-N	5.36	128.46	120.31
10	BJ	58	ASN	C-N-CA	5.36	128.46	120.31
13	BM	91	HIS	CA-C-N	5.36	129.80	120.68
13	BM	91	HIS	C-N-CA	5.36	129.80	120.68
34	CG	149	ARG	CA-C-N	5.36	127.72	120.38
34	CG	149	ARG	C-N-CA	5.36	127.72	120.38
31	CA	271	G	P-O3'-C3'	5.36	128.24	120.20
48	CV	28	VAL	N-CA-CB	5.36	118.61	111.64
8	BH	33	LYS	CA-C-N	5.36	127.31	120.56
8	BH	33	LYS	C-N-CA	5.36	127.31	120.56
54	DA	807	U	C4'-C3'-C2'	-5.35	97.25	102.60
29	CC	13	ARG	CA-C-N	5.35	127.71	120.38
29	CC	13	ARG	C-N-CA	5.35	127.71	120.38
2	AB	124	GLY	CA-C-N	5.35	131.76	121.54
2	AB	124	GLY	C-N-CA	5.35	131.76	121.54
28	CB	15	A	O4'-C1'-N9	5.35	116.22	108.20
4	BD	39	GLY	CA-C-N	5.35	127.39	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BD	39	GLY	C-N-CA	5.35	127.39	120.44
29	CC	204	VAL	N-CA-CB	5.35	120.24	111.58
7	BG	18	PHE	CA-CB-CG	5.34	119.14	113.80
16	BP	36	VAL	N-CA-CB	-5.34	105.22	112.16
13	BM	86	TYR	CA-C-N	5.33	127.95	120.28
13	BM	86	TYR	C-N-CA	5.33	127.95	120.28
45	CS	51	VAL	N-CA-C	-5.33	102.99	109.01
16	BP	79	ASN	CA-C-N	5.32	131.71	121.54
16	BP	79	ASN	C-N-CA	5.32	131.71	121.54
34	DG	149	ARG	CA-C-N	5.32	127.67	120.38
34	DG	149	ARG	C-N-CA	5.32	127.67	120.38
12	AL	72	HIS	CA-C-N	5.32	128.40	120.31
12	AL	72	HIS	C-N-CA	5.32	128.40	120.31
32	DE	198	GLU	CA-C-N	5.32	127.35	120.44
32	DE	198	GLU	C-N-CA	5.32	127.35	120.44
2	AB	204	ASP	CA-CB-CG	5.32	117.92	112.60
2	BB	124	GLY	CA-C-N	5.32	131.70	121.54
2	BB	124	GLY	C-N-CA	5.32	131.70	121.54
33	CF	23	ASN	CA-CB-CG	5.32	117.92	112.60
48	DV	53	ASN	N-CA-C	-5.31	105.44	112.24
30	CD	108	ASP	CA-CB-CG	5.30	117.90	112.60
1	AA	413	G	C1'-O4'-C4'	-5.30	104.40	109.70
31	CA	2326	C	C4'-C3'-O3'	5.30	117.34	109.40
51	CY	60	ASP	CA-CB-CG	5.29	117.89	112.60
12	AL	42	PRO	CA-C-N	5.29	130.59	120.97
12	AL	42	PRO	C-N-CA	5.29	130.59	120.97
31	CA	2225	A	C2'-C3'-O3'	5.28	117.42	109.50
16	BP	43	ALA	N-CA-C	5.27	117.44	111.11
48	DV	29	LEU	CA-C-N	5.27	128.08	120.38
48	DV	29	LEU	C-N-CA	5.27	128.08	120.38
13	AM	86	TYR	CA-C-N	5.27	127.87	120.28
13	AM	86	TYR	C-N-CA	5.27	127.87	120.28
39	CM	30	THR	N-CA-CB	5.27	119.39	110.49
12	BL	72	HIS	CA-C-N	5.26	128.31	120.31
12	BL	72	HIS	C-N-CA	5.26	128.31	120.31
20	AT	23	SER	CA-C-N	5.26	127.59	120.44
20	AT	23	SER	C-N-CA	5.26	127.59	120.44
18	AR	25	ASP	CA-CB-CG	5.26	117.86	112.60
5	BE	41	ASP	CA-CB-CG	5.26	117.86	112.60
5	AE	159	LYS	N-CA-C	-5.25	101.55	109.85
3	BC	120	ILE	CA-C-N	5.25	127.26	120.44
3	BC	120	ILE	C-N-CA	5.25	127.26	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	CE	198	GLU	CA-C-N	5.25	127.26	120.44
32	CE	198	GLU	C-N-CA	5.25	127.26	120.44
3	BC	206	GLU	CA-C-N	5.24	131.13	121.70
3	BC	206	GLU	C-N-CA	5.24	131.13	121.70
41	DO	2	ARG	N-CA-CB	-5.24	103.00	110.80
50	DX	14	ARG	CA-C-N	5.23	132.52	121.91
50	DX	14	ARG	C-N-CA	5.23	132.52	121.91
40	CN	111	GLU	CB-CG-CD	5.22	121.48	112.60
3	AC	206	GLU	CA-C-N	5.22	131.10	121.70
3	AC	206	GLU	C-N-CA	5.22	131.10	121.70
47	CU	9	LYS	CA-C-N	5.22	127.24	120.56
47	CU	9	LYS	C-N-CA	5.22	127.24	120.56
3	AC	26	THR	CA-C-N	5.21	127.22	120.44
3	AC	26	THR	C-N-CA	5.21	127.22	120.44
4	AD	143	VAL	N-CA-CB	5.21	117.24	110.99
33	CF	59	ALA	CA-C-N	5.21	127.12	120.56
33	CF	59	ALA	C-N-CA	5.21	127.12	120.56
3	AC	120	ILE	CA-C-N	5.21	127.21	120.44
3	AC	120	ILE	C-N-CA	5.21	127.21	120.44
53	DI	21	GLY	N-CA-C	5.21	118.94	112.64
4	BD	154	ARG	CA-C-N	5.20	127.11	120.56
4	BD	154	ARG	C-N-CA	5.20	127.11	120.56
29	CC	264	ASP	CA-CB-CG	5.20	117.80	112.60
31	CA	2095	A	C5'-C4'-C3'	-5.19	108.21	116.00
50	DX	42	GLY	N-CA-C	-5.18	106.77	112.99
40	DN	101	VAL	N-CA-C	-5.17	100.88	108.54
18	AR	72	ASP	CA-CB-CG	5.17	117.77	112.60
37	DK	71	ASP	CA-CB-CG	5.17	117.77	112.60
51	CY	16	ASN	CA-CB-CG	5.16	117.76	112.60
42	DP	19	GLN	CA-C-N	5.16	127.19	120.28
42	DP	19	GLN	C-N-CA	5.16	127.19	120.28
49	DW	67	GLY	CA-C-N	5.16	128.17	120.90
49	DW	67	GLY	C-N-CA	5.16	128.17	120.90
48	CV	29	LEU	CA-C-N	5.15	127.91	120.38
48	CV	29	LEU	C-N-CA	5.15	127.91	120.38
4	AD	131	ASN	CA-CB-CG	5.15	117.75	112.60
4	BD	33	LYS	CA-C-N	5.15	127.79	120.53
4	BD	33	LYS	C-N-CA	5.15	127.79	120.53
5	BE	51	GLY	CA-C-N	5.15	130.65	122.62
5	BE	51	GLY	C-N-CA	5.15	130.65	122.62
4	AD	33	LYS	CA-C-N	5.15	127.79	120.53
4	AD	33	LYS	C-N-CA	5.15	127.79	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	DR	91	ASP	CA-CB-CG	5.14	117.75	112.60
49	DW	54	ALA	CA-C-N	5.13	127.87	120.38
49	DW	54	ALA	C-N-CA	5.13	127.87	120.38
7	AG	62	PHE	CA-C-N	5.13	127.15	120.28
7	AG	62	PHE	C-N-CA	5.13	127.15	120.28
49	CW	54	ALA	CA-C-N	5.13	127.86	120.38
49	CW	54	ALA	C-N-CA	5.13	127.86	120.38
32	DE	122	GLU	CB-CG-CD	5.13	121.32	112.60
10	AJ	58	ASN	CA-C-N	5.12	128.10	120.31
10	AJ	58	ASN	C-N-CA	5.12	128.10	120.31
21	BU	47	ARG	CA-C-N	5.12	127.14	120.28
21	BU	47	ARG	C-N-CA	5.12	127.14	120.28
44	CR	31	VAL	N-CA-CB	-5.12	105.22	111.21
49	CW	67	GLY	CA-C-N	5.12	127.98	120.71
49	CW	67	GLY	C-N-CA	5.12	127.98	120.71
17	BQ	78	VAL	CA-C-N	5.12	127.01	120.56
17	BQ	78	VAL	C-N-CA	5.12	127.01	120.56
17	AQ	78	VAL	CA-C-N	5.11	127.00	120.56
17	AQ	78	VAL	C-N-CA	5.11	127.00	120.56
29	DC	13	ARG	CA-C-N	5.11	127.38	120.38
29	DC	13	ARG	C-N-CA	5.11	127.38	120.38
16	AP	76	LYS	CA-C-N	5.11	127.12	120.28
16	AP	76	LYS	C-N-CA	5.11	127.12	120.28
10	BJ	90	LEU	CA-C-N	5.11	131.29	121.54
10	BJ	90	LEU	C-N-CA	5.11	131.29	121.54
30	DD	108	ASP	CA-CB-CG	5.11	117.71	112.60
26	C5	19	ARG	CA-C-N	5.10	131.28	121.54
26	C5	19	ARG	C-N-CA	5.10	131.28	121.54
10	AJ	19	ASP	CA-CB-CG	5.09	117.69	112.60
40	CN	69	PRO	CA-C-O	-5.09	111.33	120.60
41	DO	101	GLY	CA-C-N	5.09	129.92	122.39
41	DO	101	GLY	C-N-CA	5.09	129.92	122.39
37	DK	89	PHE	CA-C-N	5.08	127.35	120.38
37	DK	89	PHE	C-N-CA	5.08	127.35	120.38
17	AQ	48	ASP	CA-CB-CG	5.08	117.68	112.60
46	CT	64	ALA	CA-C-N	5.08	131.25	121.54
46	CT	64	ALA	C-N-CA	5.08	131.25	121.54
31	CA	2035	G	C1'-O4'-C4'	-5.08	104.62	109.70
32	CE	82	GLY	CA-C-N	5.08	131.10	121.97
32	CE	82	GLY	C-N-CA	5.08	131.10	121.97
33	DF	8	TYR	CA-C-N	5.08	127.04	120.44
33	DF	8	TYR	C-N-CA	5.08	127.04	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	DY	16	ASN	CA-CB-CG	5.08	117.68	112.60
23	C2	50	LYS	CA-C-N	5.07	131.23	121.54
23	C2	50	LYS	C-N-CA	5.07	131.23	121.54
51	CY	17	ASN	CA-CB-CG	5.07	117.67	112.60
34	DG	143	GLN	CA-C-N	5.07	126.94	120.56
34	DG	143	GLN	C-N-CA	5.07	126.94	120.56
13	BM	66	GLU	CA-C-N	5.06	125.60	119.98
13	BM	66	GLU	C-N-CA	5.06	125.60	119.98
43	CQ	3	ASN	CA-C-N	5.06	126.94	120.56
43	CQ	3	ASN	C-N-CA	5.06	126.94	120.56
29	CC	121	ASP	CA-CB-CG	5.06	117.66	112.60
2	AB	142	GLU	CA-C-N	5.06	127.01	120.44
2	AB	142	GLU	C-N-CA	5.06	127.01	120.44
35	CH	52	ALA	CA-C-N	5.05	127.05	120.28
35	CH	52	ALA	C-N-CA	5.05	127.05	120.28
13	BM	6	GLY	CA-C-N	5.04	131.04	121.97
13	BM	6	GLY	C-N-CA	5.04	131.04	121.97
21	AU	33	ARG	CA-C-N	5.04	127.03	120.28
21	AU	33	ARG	C-N-CA	5.04	127.03	120.28
7	BG	62	PHE	CA-C-N	5.04	127.03	120.28
7	BG	62	PHE	C-N-CA	5.04	127.03	120.28
18	BR	25	ASP	CA-CB-CG	5.03	117.63	112.60
45	DS	47	VAL	N-CA-C	5.03	115.34	107.99
40	CN	101	VAL	N-CA-C	-5.03	101.10	108.54
5	AE	41	ASP	CA-CB-CG	5.03	117.63	112.60
1	BA	842	U	C2'-C3'-O3'	5.03	117.04	109.50
29	CC	58	HIS	N-CA-C	5.03	117.33	110.24
31	CA	686	U	O5'-C5'-C4'	-5.03	104.16	111.70
5	BE	109	GLY	CA-C-N	5.01	131.12	121.54
5	BE	109	GLY	C-N-CA	5.01	131.12	121.54
15	AO	88	ARG	N-CA-C	-5.01	100.99	108.96
4	BD	143	VAL	N-CA-CB	5.01	117.00	110.99
16	BP	76	LYS	CA-C-N	5.00	126.98	120.28
16	BP	76	LYS	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	BA	1432	G	Sidechain
1	BA	898	G	Sidechain
31	CA	2267	A	Sidechain
31	CA	2444	G	Sidechain
31	CA	250	G	Sidechain
31	CA	463	G	Sidechain
31	CA	555	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	757	G	Sidechain
40	CN	69	PRO	Mainchain
54	DA	1142	A	Sidechain
54	DA	1212	G	Sidechain
54	DA	1283	G	Sidechain
54	DA	1324	G	Sidechain
54	DA	15	G	Sidechain
54	DA	1631	G	Sidechain
54	DA	1681	G	Sidechain
54	DA	1753	G	Sidechain
54	DA	1761	C	Sidechain
54	DA	177	G	Sidechain
54	DA	1937	A	Sidechain
54	DA	1938	A	Sidechain
54	DA	1954	G	Sidechain
54	DA	221	A	Sidechain
54	DA	2250	G	Sidechain
54	DA	2267	A	Sidechain
54	DA	2323	G	Sidechain
54	DA	2375	G	Sidechain
54	DA	2481	G	Sidechain
54	DA	249	C	Sidechain
54	DA	250	G	Sidechain
54	DA	2529	G	Sidechain
54	DA	2578	G	Sidechain
54	DA	2595	G	Sidechain
54	DA	2645	G	Sidechain
54	DA	2719	G	Sidechain
54	DA	2727	A	Sidechain
54	DA	2728	U	Sidechain
54	DA	2835	A	Sidechain
54	DA	2848	G	Sidechain
54	DA	463	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
54	DA	512	G	Sidechain
54	DA	515	A	Sidechain
54	DA	555	G	Sidechain
54	DA	670	A	Sidechain
54	DA	704	G	Sidechain
54	DA	726	G	Sidechain
54	DA	858	G	Sidechain
54	DA	956	G	Sidechain
54	DA	983	A	Sidechain
54	DA	984	A	Sidechain
40	DN	69	PRO	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32933	0	16592	109	0
1	BA	32911	0	16581	112	0
2	AB	1753	0	1780	7	0
2	BB	1753	0	1780	9	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	11	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	14	0
5	BE	1105	0	1148	25	0
6	AF	862	0	864	8	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	7	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	8	0
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	13	0
11	BK	877	0	887	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	957	0	1017	6	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	14	0
13	BM	884	0	941	19	0
14	AN	805	0	844	9	0
14	BN	805	0	844	8	0
15	AO	714	0	734	0	0
15	BO	714	0	734	0	0
16	AP	649	0	666	2	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	13	0
18	AR	456	0	478	4	0
18	BR	456	0	478	2	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	3	0
20	BT	665	0	714	5	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	5	0
22	D1	444	0	458	9	0
23	C2	409	0	440	6	0
23	D2	414	0	442	6	0
24	C3	377	0	418	3	0
24	D3	377	0	418	3	0
25	C4	504	0	572	2	0
25	D4	504	0	572	2	0
26	C5	302	0	340	6	0
26	D5	302	0	340	2	0
27	C0	449	0	488	3	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	6	0
28	DB	2569	0	1301	3	0
29	CC	2083	0	2154	24	0
29	DC	2083	0	2154	13	0
30	CD	1565	0	1614	15	0
30	DD	1576	0	1627	15	0
31	CA	62229	0	31318	226	0
32	CE	1552	0	1619	19	0
32	DE	1552	0	1619	9	0
33	CF	1411	0	1444	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DF	1411	0	1444	12	0
34	CG	1323	0	1371	8	0
34	DG	1323	0	1371	8	0
35	CH	1110	0	1148	11	0
35	DH	1110	0	1148	10	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	5	0
37	CK	1129	0	1162	10	0
37	DK	1129	0	1162	5	0
38	CL	938	0	1012	10	0
38	DL	946	0	1023	10	0
39	CM	1053	0	1129	19	0
39	DM	1053	0	1129	6	0
40	CN	1075	0	1154	9	0
40	DN	1092	0	1177	13	0
41	CO	960	0	1000	6	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	11	0
43	CQ	917	0	962	6	0
43	DQ	917	0	962	7	0
44	CR	947	0	1019	11	0
44	DR	947	0	1019	13	0
45	CS	816	0	839	12	0
45	DS	816	0	839	7	0
46	CT	857	0	922	10	0
46	DT	857	0	922	10	0
47	CU	739	0	807	8	0
47	DU	739	0	807	7	0
48	CV	780	0	831	7	0
48	DV	780	0	831	6	0
49	CW	753	0	780	5	0
49	DW	753	0	780	4	0
50	CX	569	0	581	3	0
50	DX	591	0	606	10	0
51	CY	625	0	652	8	0
51	DY	625	0	652	5	0
52	CZ	501	0	531	3	0
52	DZ	501	0	531	2	0
53	DI	1023	0	1052	15	0
54	DA	62423	0	31411	176	0
55	AA	72	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BA	45	0	0	0	0
55	CA	156	0	0	0	0
55	CB	3	0	0	0	0
55	DA	183	0	0	0	0
55	DB	9	0	0	0	0
55	DD	1	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	1	0
56	DA	26	0	36	3	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	3	0
57	AA	16	0	28	3	0
57	DA	40	0	70	3	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	66	0	132	7	0
58	DM	6	0	12	0	0
59	AA	64	1	42	2	0
59	BA	64	1	42	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	1	0
62	DB	12	0	18	0	0
63	D1	10	0	14	2	0
63	DA	60	0	84	4	0
63	DS	10	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	DU	10	0	14	3	0
64	DA	40	0	76	2	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	501	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	5	0	0	2	0
69	AN	6	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AT	3	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BK	2	0	0	0	0
69	BL	4	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BT	2	0	0	0	0
69	BU	2	0	0	0	0
69	C3	4	0	0	0	0
69	C4	1	0	0	0	0
69	CA	691	0	0	3	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CO	2	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	0	0
69	D1	43	0	0	0	0
69	D2	6	0	0	0	0
69	D3	22	0	0	0	0
69	D4	39	0	0	0	0
69	D5	8	0	0	0	0
69	DA	4840	0	0	15	0
69	DB	209	0	0	1	0
69	DC	100	0	0	1	0
69	DD	98	0	0	2	0
69	DE	61	0	0	0	0
69	DF	15	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	1	0
69	DM	63	0	0	0	0
69	DN	72	0	0	0	0
69	DO	44	0	0	0	0
69	DP	38	0	0	0	0
69	DQ	33	0	0	0	0
69	DR	62	0	0	1	0
69	DS	46	0	0	2	0
69	DT	69	0	0	1	0
69	DU	18	0	0	0	0
69	DV	20	0	0	0	0
69	DW	31	0	0	0	0
69	DX	25	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	8	0	0	0	0
All	All	295259	2	194494	1283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.27	1.10
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.61	1.00
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.46	0.97
31:CA:1847:A:HO2'	31:CA:1848:A:H8	0.98	0.95
31:CA:528:A:C2	31:CA:2043:C:H4'	2.00	0.95
54:DA:2796:U:H3	54:DA:2799:A:H61	1.11	0.95
54:DA:1847:A:HO2'	54:DA:1848:A:H8	0.98	0.94
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.50	0.94
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.02	0.94
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.34	0.93
31:CA:2796:U:H3	31:CA:2799:A:H61	1.14	0.93
39:CM:77:ILE:HD11	39:CM:108:ALA:HB1	1.50	0.92
31:CA:1936:A:H2	31:CA:1943:U:H3	0.96	0.91
14:AN:66:GLN:HB2	69:AN:206:HOH:O	1.70	0.90
45:CS:14:VAL:CG2	45:CS:98:ILE:HG13	2.00	0.90
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.53	0.89
1:AA:307:C:N4	57:AA:1676:MPD:H12	1.88	0.88
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.54	0.88
54:DA:1913:A:H4'	54:DA:1913:A:OP1	1.72	0.87
31:CA:135:U:H3	31:CA:144:A:H61	1.20	0.87
54:DA:135:U:H3	54:DA:144:A:H61	1.20	0.87
46:CT:86:MET:HB2	46:CT:96:ILE:HD11	1.54	0.86
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.59	0.85
54:DA:2255:G:H21	68:DA:3220:TRS:H12	1.42	0.85
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.58	0.84
44:DR:20:GLN:HG3	56:DR:202:PG4:H42	1.58	0.84
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.59	0.83
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.61	0.82
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.61	0.82
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.59	0.81
45:CS:14:VAL:HG21	45:CS:98:ILE:CG1	2.10	0.81
1:BA:841:C:H3'	1:BA:842:U:H5''	1.62	0.80
1:BA:664:G:H22	1:BA:741:G:H1	1.29	0.80
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.46	0.80
31:CA:1779:U:H5	31:CA:1784:A:N7	1.80	0.79
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.63	0.79
1:BA:1052:G:H22	1:BA:1206:G:H1	1.30	0.79
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.65	0.78
1:AA:1305:G:H21	1:AA:1332:A:H2	1.32	0.78
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.48	0.78
44:DR:28:ARG:HD3	69:DR:302:HOH:O	1.85	0.77
1:AA:664:G:H22	1:AA:741:G:H1	1.31	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1936:A:H2	31:CA:1943:U:N3	1.80	0.77
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.67	0.77
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.67	0.76
32:DE:33:VAL:HG22	57:DA:3192:MPD:H12	1.66	0.76
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.68	0.76
1:BA:1305:G:H21	1:BA:1332:A:H2	1.32	0.76
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.67	0.75
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.33	0.75
31:CA:846:U:H1'	31:CA:847:U:H5	1.52	0.74
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.69	0.74
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.68	0.73
38:DL:113:MET:HE1	38:DL:116:ILE:HD11	1.72	0.72
54:DA:2127:G:H4'	54:DA:2128:G:OP1	1.89	0.72
1:BA:841:C:H3'	1:BA:842:U:C5'	2.19	0.72
54:DA:568:U:H1'	54:DA:2030:6MZ:H9C1	1.72	0.71
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.71	0.71
69:DD:443:HOH:O	54:DA:1671:U:H4'	1.90	0.71
34:CG:24:ILE:HD11	34:CG:43:VAL:HG11	1.71	0.71
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.56	0.71
34:DG:24:ILE:HD11	34:DG:43:VAL:HG11	1.74	0.70
54:DA:1105:U:H2'	54:DA:1106:G:H8	1.56	0.70
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.74	0.70
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.07	0.69
22:C1:16:ARG:HA	31:CA:2046:G:H5'	1.73	0.69
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.28	0.69
34:CG:76:VAL:O	34:CG:80:THR:HG22	1.92	0.69
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.74	0.69
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.74	0.69
46:CT:59:GLU:HA	46:CT:64:ALA:HA	1.73	0.69
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.93	0.68
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.75	0.68
35:DH:41:LYS:HA	35:DH:44:ILE:HG12	1.76	0.68
65:DA:3202:1PE:H231	69:DA:3678:HOH:O	1.92	0.68
38:DL:70:ARG:HD3	38:DL:76:VAL:HG22	1.76	0.68
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.59	0.68
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.75	0.68
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.75	0.68
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.94	0.67
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.28	0.67
47:CU:54:GLU:HB3	47:CU:88:LYS:HD2	1.77	0.67
35:CH:41:LYS:HA	35:CH:44:ILE:HG12	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.59	0.67
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.75	0.67
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.77	0.67
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.09	0.67
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.30	0.67
54:DA:2033:A:H5'	69:DA:3362:HOH:O	1.96	0.66
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.29	0.66
69:DK:315:HOH:O	44:DR:93:LYS:HD2	1.93	0.66
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.78	0.66
35:CH:15:LEU:HD22	35:CH:15:LEU:H	1.60	0.66
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.60	0.66
47:DU:54:GLU:HB3	47:DU:88:LYS:HD2	1.77	0.66
46:CT:73:LYS:HB2	46:CT:106:VAL:HB	1.78	0.66
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.60	0.66
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.95	0.66
25:D4:8:ARG:HD3	54:DA:245:G:O6	1.96	0.66
48:CV:7:ARG:O	48:CV:25:VAL:HB	1.95	0.66
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.32	0.65
5:AE:157:ARG:HD2	8:AH:43:GLU:O	1.95	0.65
42:DP:39:VAL:HB	42:DP:49:VAL:HG23	1.77	0.65
31:CA:528:A:H2	31:CA:2043:C:H4'	1.57	0.65
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.32	0.65
40:CN:41:LEU:HD21	40:CN:124:LEU:HD22	1.78	0.65
54:DA:1105:U:H2'	54:DA:1106:G:C8	2.30	0.65
39:CM:21:ARG:CG	39:CM:21:ARG:HH21	2.09	0.65
31:CA:528:A:H2'	31:CA:529:A:H5''	1.77	0.65
39:CM:82:LEU:HD11	39:CM:116:VAL:HG23	1.78	0.65
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.45	0.65
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.80	0.64
31:CA:674:G:H1'	32:CE:69:ARG:HH11	1.62	0.64
31:CA:1311:G:H21	31:CA:1603:A:H62	1.44	0.64
58:DA:3195:PUT:H21	69:DA:5832:HOH:O	1.96	0.64
44:DR:20:GLN:CG	56:DR:202:PG4:H42	2.26	0.64
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.79	0.64
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.43	0.64
46:DT:73:LYS:HB2	46:DT:106:VAL:HB	1.79	0.64
54:DA:2128:G:H1	54:DA:2160:C:H42	1.44	0.64
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.25	0.63
40:DN:18[B]:ARG:HG3	28:DB:90:C:H5''	1.79	0.63
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.80	0.63
34:CG:80:THR:HG23	34:CG:81:GLU:H	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1853:A:N1	54:DA:2087:G:H1'	2.14	0.63
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.98	0.63
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.81	0.62
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.64	0.62
54:DA:45:G:H5''	54:DA:46:G:H5'	1.82	0.62
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.82	0.62
1:BA:1012:A:H61	1:BA:1017:U:H3	1.48	0.62
31:CA:1131:G:OP1	37:CK:82:GLY:HA2	1.99	0.61
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.81	0.61
33:CF:36:LEU:HD21	33:CF:91:LEU:HD11	1.82	0.61
1:AA:1012:A:H61	1:AA:1017:U:H3	1.49	0.61
48:DV:52:LEU:HB3	48:DV:54:GLN:HB2	1.81	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.10	0.61
38:CL:43:ILE:HD12	38:CL:56:ASP:HB2	1.82	0.61
41:CO:33:ILE:HD12	41:CO:114:GLU:HB3	1.82	0.61
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:HH11	1.64	0.61
31:CA:45:G:H5''	31:CA:46:G:H5'	1.82	0.61
31:CA:118:A:N3	31:CA:178:G:H1'	2.16	0.60
46:CT:17:VAL:HG11	46:CT:103:ILE:HG12	1.83	0.60
45:DS:83:TYR:CE1	54:DA:1187:G:H5''	2.36	0.60
31:CA:784:G:H5'	31:CA:785:G:OP1	2.01	0.60
40:DN:77:PRO:HG2	40:DN:80:VAL:HG21	1.84	0.60
46:DT:17:VAL:HG11	46:DT:103:ILE:HG12	1.83	0.60
54:DA:2256:G:H21	56:DA:3193:PG4:H31	1.67	0.60
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.37	0.60
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.67	0.60
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.48	0.60
30:DD:114:LYS:HE2	54:DA:2681:C:OP2	2.02	0.60
47:CU:18:GLU:H	47:CU:18:GLU:CD	2.08	0.60
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.02	0.60
53:DI:69:PHE:HB3	53:DI:72:LEU:HD12	1.83	0.60
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.84	0.60
38:DL:113:MET:CE	38:DL:116:ILE:HD11	2.32	0.60
1:AA:1396:A:H3'	59:AA:1681:TAC:H433	1.84	0.59
31:CA:674:G:H1'	32:CE:69:ARG:HD2	1.85	0.59
42:DP:31:THR:HG21	28:DB:28:C:OP1	2.02	0.59
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.67	0.59
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.37	0.59
48:CV:13:VAL:HG21	48:CV:39:ILE:HG21	1.85	0.59
38:DL:43:ILE:HD12	38:DL:56:ASP:HB2	1.84	0.59
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:108:G:H5''	1:BA:108:G:N3	2.18	0.59
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.85	0.59
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	1.84	0.59
31:CA:457:A:N1	31:CA:470:A:H5''	2.17	0.59
41:DO:33:ILE:HD12	41:DO:114:GLU:HB3	1.83	0.59
43:DQ:53:ARG:NH2	54:DA:2720:U:OP1	2.36	0.59
39:CM:79:LEU:HD11	39:CM:112:LEU:HD12	1.84	0.59
44:CR:112:LYS:HD3	45:CS:48:LYS:HG3	1.84	0.59
48:CV:45:HIS:HD2	48:CV:58:ILE:HG12	1.68	0.59
48:DV:13:VAL:HG21	48:DV:39:ILE:HG21	1.84	0.59
54:DA:2796:U:H3	54:DA:2799:A:N6	1.92	0.59
31:CA:910:A:H62	40:CN:12:MET:HA	1.67	0.59
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.49	0.59
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.03	0.59
1:AA:108:G:N3	1:AA:108:G:H5''	2.17	0.59
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.85	0.59
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.85	0.59
37:CK:81:ILE:HG23	37:CK:82:GLY:H	1.67	0.59
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.85	0.58
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.86	0.58
50:DX:21:LEU:HD11	50:DX:41[A]:ARG:HE	1.68	0.58
31:CA:974:G:H8	31:CA:990:A:H62	1.52	0.58
31:CA:206:U:H2'	31:CA:207:A:H8	1.69	0.58
30:DD:186:LEU:HD21	43:DQ:4:ILE:HG21	1.85	0.58
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.86	0.58
31:CA:2796:U:H3	31:CA:2799:A:N6	1.94	0.58
54:DA:62:U:O4'	57:DA:3204:MPD:H31	2.03	0.58
50:CX:37:ILE:HG21	50:CX:80:ILE:HG21	1.85	0.58
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.85	0.58
39:CM:77:ILE:CD1	39:CM:108:ALA:HB1	2.29	0.58
30:DD:99:GLU:HG2	30:DD:182:ALA:HB2	1.86	0.58
50:DX:41[A]:ARG:HH11	50:DX:41[A]:ARG:HG2	1.69	0.58
46:CT:82:MET:HB2	46:CT:98:LYS:HB2	1.85	0.57
48:CV:74:ASN:HD22	48:CV:77:THR:H	1.51	0.57
43:DQ:29:LYS:HB3	43:DQ:40:LEU:HD13	1.85	0.57
46:DT:82:MET:HB2	46:DT:98:LYS:HB2	1.86	0.57
47:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.85	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.85	0.57
30:DD:140:HIS:HB3	69:DD:487:HOH:O	2.02	0.57
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.39	0.57
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.86	0.57
35:CH:4:ILE:HD11	35:CH:44:ILE:HG22	1.86	0.57
38:CL:58:LEU:HD11	38:CL:86:LEU:HD13	1.86	0.57
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.57
54:DA:1975:G:H21	63:DA:3225:PGE:C2	2.18	0.57
31:CA:1936:A:H62	31:CA:1963:U:H3	1.50	0.57
50:DX:59:LEU:HD12	50:DX:80:ILE:HD12	1.87	0.57
54:DA:1417:C:H5'	54:DA:1588:G:H1'	1.87	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.85	0.57
24:D3:19:ARG:HD3	54:DA:125:A:OP2	2.04	0.57
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.87	0.57
20:BT:28:MET:HE1	20:BT:67:ILE:HG12	1.87	0.57
1:AA:86:G:H21	1:AA:87:C:H41	1.53	0.57
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.40	0.57
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.86	0.57
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.86	0.57
42:DP:31:THR:HG22	42:DP:34:HIS:H	1.69	0.57
1:AA:774:G:H21	56:AA:1670:PG4:H51	1.70	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.87	0.56
42:CP:31:THR:HG22	42:CP:34:HIS:H	1.69	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
1:BA:202:G:H1	1:BA:215:C:H42	1.51	0.56
33:CF:31:VAL:CG1	33:CF:97:TRP:CH2	2.88	0.56
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.88	0.56
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.86	0.56
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.87	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.87	0.56
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.86	0.56
31:CA:1156:A:H5''	69:CA:3399:HOH:O	2.05	0.56
50:DX:37:ILE:HG21	50:DX:80:ILE:HG21	1.87	0.56
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.86	0.56
31:CA:244:A:H5''	39:CM:67:THR:HG21	1.87	0.56
54:DA:1746:A:H2'	54:DA:1747:U:C6	2.41	0.56
1:AA:81:A:H61	1:AA:86:G:H1	1.54	0.56
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.20	0.56
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.87	0.56
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.40	0.56
54:DA:526:A:H2'	69:DA:3716:HOH:O	2.05	0.56
54:DA:1975:G:H21	63:DA:3225:PGE:H22	1.70	0.56
25:C4:54:ASP:HB3	39:CM:57:LEU:HD22	1.86	0.56
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:16:VAL:HG13	11:BK:79:ILE:HG13	1.88	0.56
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.88	0.56
22:D1:4:GLN:HA	54:DA:2615:U:C2	2.41	0.56
36:CJ:19:ASN:H	36:CJ:20:PRO:HD2	1.71	0.56
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.87	0.56
38:DL:58:LEU:HD11	38:DL:86:LEU:HD13	1.88	0.56
1:AA:137:U:H3	1:AA:226:G:H1	1.53	0.56
1:AA:209:U:H4'	1:AA:210:C:OP2	2.06	0.56
17:BQ:19:LYS:HG2	17:BQ:49:GLU:HA	1.87	0.56
31:CA:2019:A:H4'	44:CR:34:VAL:HG21	1.88	0.56
40:CN:77:PRO:HG2	40:CN:80:VAL:HG21	1.87	0.56
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.06	0.55
22:D1:9:THR:CG2	54:DA:2020:A:H5'	2.36	0.55
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.06	0.55
32:DE:189:THR:HG22	32:DE:192:ALA:H	1.71	0.55
1:AA:202:G:H1	1:AA:215:C:H42	1.54	0.55
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.88	0.55
48:DV:45:HIS:HD2	48:DV:58:ILE:HG12	1.71	0.55
1:BA:240:G:H4'	1:BA:240:G:OP1	2.06	0.55
31:CA:396:G:H1'	51:CY:29:PHE:HB3	1.87	0.55
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.55
32:DE:48:THR:HG22	32:DE:86:ALA:HB3	1.88	0.55
44:DR:6:ARG:NH1	54:DA:585:G:N7	2.53	0.55
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.07	0.55
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.36	0.55
38:CL:35:VAL:HG12	38:CL:106:GLU:HG2	1.87	0.55
50:CX:59:LEU:HD12	50:CX:80:ILE:HD12	1.87	0.55
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.89	0.55
1:BA:137:U:H3	1:BA:226:G:H1	1.54	0.55
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.88	0.55
31:CA:460:A:H5'	47:CU:73:ARG:HH22	1.72	0.55
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.87	0.55
36:DJ:19:ASN:H	36:DJ:20:PRO:HD2	1.71	0.55
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.41	0.55
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:NH1	2.22	0.55
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.71	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.89	0.55
1:BA:374:A:H5''	1:BA:452:A:C2	2.41	0.55
12:BL:80:ILE:HD12	12:BL:97:THR:CG2	2.30	0.55
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.89	0.55
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CE:3:LEU:HD12	32:CE:14:VAL:HG11	1.89	0.55
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	1.89	0.54
31:CA:699:A:H2'	31:CA:700:G:O4'	2.07	0.54
46:CT:66:ILE:HA	46:CT:69:LEU:HD22	1.89	0.54
1:AA:1144:G:H21	1:AA:1146:A:H62	1.54	0.54
31:CA:247:G:H4'	31:CA:386:G:C5	2.41	0.54
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.42	0.54
45:CS:78:ARG:HB2	45:CS:83:TYR:HD1	1.71	0.54
54:DA:789:A:OP1	58:DA:3222:PUT:H11	2.07	0.54
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.54
31:CA:863:A:H2'	31:CA:864:G:C8	2.42	0.54
54:DA:2065:C:H4'	54:DA:2251:OMG:HM22	1.89	0.54
54:DA:1482:G:H1'	54:DA:1509:A:H61	1.73	0.54
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.07	0.54
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.54
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.73	0.54
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.88	0.54
28:CB:55:U:H1'	33:CF:26:MET:HG3	1.88	0.54
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.42	0.54
1:BA:1144:G:H21	1:BA:1146:A:H62	1.54	0.54
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.89	0.54
63:D1:102:PGE:H4	69:DT:311:HOH:O	2.08	0.54
32:CE:149:ILE:HG12	32:CE:188:MET:HG2	1.90	0.54
52:CZ:56:LEU:HA	52:CZ:59:GLU:HG2	1.89	0.54
54:DA:1180:U:H5''	54:DA:1180:U:H6	1.73	0.54
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.89	0.54
32:DE:3:LEU:HD12	32:DE:14:VAL:HG11	1.90	0.54
41:DO:2:ARG:HG3	54:DA:1653:G:H3'	1.90	0.54
1:AA:412:A:H3'	1:AA:413:G:H5'	1.90	0.54
1:AA:307:C:N4	57:AA:1676:MPD:C1	2.68	0.53
31:CA:550:C:H2'	31:CA:551:G:H5''	1.90	0.53
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.53
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.38	0.53
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.08	0.53
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.08	0.53
33:CF:61:SER:HB2	33:CF:91:LEU:HD21	1.90	0.53
54:DA:1847:A:O2'	54:DA:1848:A:H8	1.78	0.53
1:AA:73:C:HO2'	1:AA:74:A:H8	1.56	0.53
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.90	0.53
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.89	0.53
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:CU:69:ARG:HB2	47:CU:74:ILE:HG22	1.90	0.53
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.90	0.53
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.43	0.53
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.23	0.53
31:CA:782:A:H5'	31:CA:783:A:C2	2.44	0.53
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.73	0.53
33:DF:61:SER:HB2	33:DF:91:LEU:HD21	1.90	0.53
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	1.89	0.53
1:BA:374:A:H5''	1:BA:452:A:N1	2.23	0.53
46:CT:69:LEU:HG	46:CT:107:VAL:HG22	1.91	0.53
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.91	0.53
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.90	0.53
24:D3:2:LYS:HE2	54:DA:687:C:H5''	1.90	0.53
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.53
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.42	0.53
46:CT:29:VAL:HG22	46:CT:51:LEU:HD11	1.89	0.53
33:DF:132:VAL:HG22	33:DF:152:LEU:HG	1.91	0.53
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.23	0.53
31:CA:1363:C:H2'	31:CA:1364:G:C8	2.44	0.53
32:CE:189:THR:HG22	32:CE:192:ALA:H	1.73	0.53
33:CF:44:ILE:HG21	33:CF:79:ILE:HG22	1.91	0.53
37:DK:9:GLU:HG2	69:DA:5751:HOH:O	2.09	0.53
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.34	0.52
34:DG:17:VAL:HG11	34:DG:50:LEU:HD21	1.90	0.52
1:BA:209:U:H4'	1:BA:210:C:OP2	2.08	0.52
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	1.91	0.52
30:DD:152:PRO:HG3	30:DD:156:PHE:CZ	2.45	0.52
56:DS:202:PG4:H21	69:DS:315:HOH:O	2.09	0.52
54:DA:550:C:H2'	54:DA:551:G:H5''	1.91	0.52
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.91	0.52
1:BA:12:U:H4'	1:BA:526:C:H4'	1.91	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.91	0.52
34:CG:17:VAL:HG11	34:CG:50:LEU:HD21	1.90	0.52
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.22	0.52
17:BQ:8:LEU:HD23	17:BQ:25:ILE:HG21	1.92	0.52
35:DH:4:ILE:HD11	35:DH:44:ILE:HG22	1.91	0.52
53:DI:8:LYS:O	53:DI:12:VAL:HG23	2.09	0.52
1:AA:1126:U:O2	1:AA:1280:A:H5'	2.09	0.52
41:CO:73:ASN:HA	41:CO:76:VAL:HG13	1.92	0.52
33:DF:44:ILE:HG21	33:DF:79:ILE:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:28:C:OP1	42:CP:31:THR:HG21	2.10	0.52
31:CA:2718:G:OP1	43:CQ:98:TYR:HD2	1.93	0.52
32:CE:48:THR:HG22	32:CE:86:ALA:HB3	1.91	0.52
50:DX:18:ALA:HB3	50:DX:20:ARG:NH1	2.24	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.44	0.52
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.45	0.52
54:DA:2291:U:H2'	54:DA:2292:U:C6	2.45	0.52
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.91	0.52
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.91	0.52
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.24	0.52
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.75	0.52
54:DA:551:G:H5''	54:DA:551:G:H8	1.75	0.52
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.91	0.52
1:BA:1126:U:O2	1:BA:1280:A:H5'	2.09	0.52
1:BA:1343:G:H2'	1:BA:1344:C:C6	2.44	0.52
31:CA:846:U:H1'	31:CA:847:U:C5	2.40	0.52
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.45	0.52
38:CL:121:GLU:HG2	38:CL:122:VAL:HG23	1.92	0.52
45:DS:16:GLU:HG2	45:DS:100:GLY:HA2	1.92	0.52
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.91	0.51
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.91	0.51
31:CA:566:U:O4	45:CS:80:ARG:HD3	2.10	0.51
37:CK:114:LEU:HG	37:CK:118:MET:HE3	1.92	0.51
54:DA:837:C:H5	69:DA:6614:HOH:O	1.93	0.51
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.51
8:AH:96:MET:HE3	8:AH:130:ALA:HB1	1.92	0.51
53:DI:132:TYR:H	53:DI:133:GLU:HB2	1.75	0.51
31:CA:784:G:H3'	69:CA:3435:HOH:O	2.10	0.51
31:CA:1363:C:H2'	31:CA:1364:G:H8	1.76	0.51
51:CY:4:VAL:HG22	51:CY:11:ARG:HG3	1.91	0.51
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.94	0.51
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.25	0.51
33:CF:36:LEU:HB2	33:CF:57:LEU:HD21	1.92	0.51
33:DF:36:LEU:HB2	33:DF:57:LEU:HD21	1.92	0.51
54:DA:793:A:OP1	64:DA:3224:SPD:H81	2.10	0.51
1:AA:528:C:H5''	1:AA:528:C:H6	1.76	0.51
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.91	0.51
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.76	0.51
8:BH:96:MET:HE2	8:BH:130:ALA:HB1	1.91	0.51
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.92	0.51
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.41	0.51
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.39	0.51
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.76	0.51
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.11	0.51
39:CM:21:ARG:HH21	39:CM:21:ARG:HG2	1.75	0.51
37:DK:56:VAL:HB	37:DK:124:VAL:HB	1.93	0.51
43:DQ:52:ASN:O	54:DA:2845:U:H5''	2.10	0.51
56:DA:3216:PG4:H31	69:DA:4497:HOH:O	2.11	0.51
13:AM:12:HIS:HB3	69:AM:305:HOH:O	2.10	0.51
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.08	0.51
40:CN:40:ARG:HD3	40:CN:93:VAL:HG21	1.93	0.51
37:DK:114:LEU:HG	37:DK:118:MET:HE3	1.91	0.51
44:DR:6:ARG:HD3	54:DA:1250:G:C5'	2.41	0.51
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.45	0.51
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.93	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
42:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.92	0.51
26:C5:2:LYS:HE3	26:C5:4:ARG:HH11	1.76	0.51
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.92	0.51
53:DI:50:VAL:HG13	53:DI:85:VAL:HG22	1.93	0.51
64:DA:3224:SPD:H82	69:DA:5291:HOH:O	2.10	0.51
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.46	0.50
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.76	0.50
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.47	0.50
32:CE:149:ILE:HD12	32:CE:172:ALA:HA	1.93	0.50
34:DG:164:TYR:HB2	34:DG:167:GLU:HB2	1.93	0.50
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.50
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.93	0.50
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.93	0.50
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.93	0.50
35:CH:1:MET:HE3	35:CH:23:ALA:HA	1.92	0.50
41:DO:73:ASN:HA	41:DO:76:VAL:HG13	1.93	0.50
1:BA:1151:A:O2'	1:BA:1152:A:H8	1.94	0.50
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.39	0.50
54:DA:12:U:H6	69:DA:4057:HOH:O	1.93	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.94	0.50
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.92	0.50
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.46	0.50
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.11	0.50
33:CF:132:VAL:HG22	33:CF:152:LEU:HG	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:781:A:H2'	31:CA:1777:U:O2'	2.11	0.50
30:DD:150[A]:MEQ:HE3	54:DA:2032:G:C8	2.47	0.50
37:CK:81:ILE:CG2	37:CK:82:GLY:H	2.24	0.50
34:DG:86:LYS:HG2	34:DG:132:VAL:HG22	1.93	0.50
46:DT:10:ALA:HB1	46:DT:46:LEU:HD13	1.94	0.50
54:DA:287:G:H1	54:DA:353:C:H42	1.60	0.50
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.47	0.50
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.45	0.50
1:BA:374:A:OP1	1:BA:452:A:N1	2.44	0.50
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.77	0.50
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.46	0.50
27:D0:45:ARG:HH12	27:D0:59:GLU:CD	2.20	0.50
31:CA:328:U:O3'	48:CV:66:GLN:HG3	2.11	0.50
35:CH:27:ARG:HH11	51:CY:60:ASP:HA	1.77	0.50
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	1.94	0.50
54:DA:2886[A]:A:C2	54:DA:2887[A]:A:H1'	2.46	0.50
1:AA:412:A:H3'	1:AA:413:G:C5'	2.42	0.50
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.94	0.50
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.47	0.50
38:CL:76:VAL:HG12	43:CQ:73:VAL:HB	1.93	0.50
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.93	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.94	0.49
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.52	0.49
35:CH:94:ILE:HB	35:CH:122:LEU:HB2	1.95	0.49
37:CK:81:ILE:HG23	37:CK:82:GLY:N	2.27	0.49
33:DF:88:LYS:HD3	54:DA:2313:C:H5''	1.93	0.49
1:BA:518:C:H2'	1:BA:530:G:C8	2.48	0.49
1:BA:1328:C:H5''	13:BM:28:THR:HG21	1.95	0.49
31:CA:593:U:H2'	31:CA:594:U:C6	2.47	0.49
54:DA:118:A:N3	54:DA:178:G:H1'	2.26	0.49
54:DA:1172:C:C5	54:DA:1173:U:H1'	2.47	0.49
54:DA:1515:A:H2'	54:DA:1516:G:O4'	2.12	0.49
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.78	0.49
53:DI:64:VAL:HG22	53:DI:69:PHE:HB2	1.95	0.49
1:AA:131:A:H2'	1:AA:132:C:C6	2.48	0.49
1:BA:845:A:O5'	1:BA:845:A:H8	1.96	0.49
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.77	0.49
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.78	0.49
30:DD:161:MET:HG2	69:DA:6194:HOH:O	2.12	0.49
36:CJ:14:ALA:HB3	36:CJ:17:MET:HB2	1.93	0.49
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.48	0.49
26:D5:25:VAL:HB	26:D5:35:GLN:HB2	1.94	0.49
31:CA:1775:U:O4	31:CA:1789:A:H2	1.95	0.49
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	1.95	0.49
30:DD:150[A]:MEQ:HG2	69:DA:3634:HOH:O	2.13	0.49
41:CO:95:THR:HG21	41:CO:113:ILE:HD11	1.94	0.49
53:DI:126:LEU:HA	53:DI:129:LEU:HD12	1.94	0.49
54:DA:136:G:H1	54:DA:143:C:H42	1.61	0.49
54:DA:593:U:H2'	54:DA:594:U:C6	2.48	0.49
31:CA:551:G:H5''	31:CA:551:G:H8	1.76	0.49
34:CG:86:LYS:HG2	34:CG:132:VAL:HG22	1.95	0.49
38:CL:103:VAL:O	38:CL:122:VAL:HB	2.13	0.49
6:AF:3:HIS:CE1	6:AF:65:GLU:HG3	2.48	0.49
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.95	0.49
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.78	0.49
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.94	0.49
41:DO:55:ALA:HA	41:DO:80:PHE:CE2	2.48	0.49
44:DR:31:VAL:HG13	54:DA:580:U:O3'	2.13	0.49
48:DV:94:ARG:HB3	48:DV:103:ILE:HD12	1.95	0.49
54:DA:2327:A:H2'	54:DA:2328:A:C8	2.48	0.49
54:DA:2813:A:C2	54:DA:2887[B]:A:N6	2.80	0.49
1:AA:439:U:H5''	4:AD:121:LYS:HD2	1.95	0.48
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.37	0.48
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.95	0.48
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.78	0.48
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	1.94	0.48
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.28	0.48
22:D1:24:ALA:HB3	63:D1:102:PGE:H5	1.95	0.48
45:CS:49:ILE:HB	45:CS:51:VAL:O	2.13	0.48
54:DA:12:U:O2	54:DA:12:U:H2'	2.13	0.48
54:DA:572:A:H5''	54:DA:573:U:OP2	2.13	0.48
54:DA:784:G:H5'	54:DA:785:G:OP1	2.13	0.48
54:DA:1536:C:H4'	54:DA:1537:G:H5''	1.94	0.48
54:DA:1773:A:H5''	69:DA:4750:HOH:O	2.12	0.48
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.95	0.48
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.78	0.48
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.78	0.48
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.78	0.48
29:CC:67:PHE:CD1	29:CC:105:LEU:HD11	2.48	0.48
31:CA:1379:U:H5'	31:CA:1379:U:H6	1.78	0.48
31:CA:1956:U:O2	31:CA:1985:C:H4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DL:1:MET:HE3	38:DL:32:TYR:CZ	2.49	0.48
40:DN:21:ALA:HB1	40:DN:100:LYS:HG2	1.95	0.48
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.79	0.48
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.95	0.48
29:CC:3:VAL:HG21	29:CC:202:LEU:HD23	1.96	0.48
31:CA:12:U:H2'	31:CA:12:U:O2	2.14	0.48
29:DC:233:GLY:HA3	69:DC:309:HOH:O	2.12	0.48
33:CF:106:ILE:HD12	33:CF:139:PRO:HG2	1.95	0.48
37:CK:56:VAL:HB	37:CK:124:VAL:HB	1.93	0.48
33:DF:131:GLY:HA3	54:DA:2305:U:H5''	1.95	0.48
35:DH:94:ILE:HB	35:DH:122:LEU:HB2	1.95	0.48
40:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.43	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.96	0.48
32:CE:108:ILE:HG22	39:CM:1:MET:SD	2.54	0.48
36:CJ:103:ARG:HA	36:CJ:106:LEU:HD12	1.95	0.48
42:DP:35:ILE:HG21	42:DP:71:ALA:HA	1.94	0.48
54:DA:1794:A:H2'	54:DA:1795:C:C6	2.47	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:H11	1.95	0.48
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.14	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.48	0.48
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.96	0.48
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.78	0.48
31:CA:287:G:H1	31:CA:353:C:H42	1.61	0.48
33:DF:106:ILE:HD12	33:DF:139:PRO:HG2	1.94	0.48
1:AA:1346:A:H61	1:AA:1374:A:H3'	1.77	0.48
13:AM:26:GLY:HA2	69:AM:303:HOH:O	2.13	0.48
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.95	0.48
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.14	0.48
36:DJ:103:ARG:HA	36:DJ:106:LEU:HD12	1.95	0.48
26:C5:25:VAL:HB	26:C5:35:GLN:HB2	1.95	0.48
1:BA:131:A:H2'	1:BA:132:C:C6	2.49	0.48
31:CA:136:G:H1	31:CA:143:C:H42	1.62	0.48
31:CA:450:G:H2'	31:CA:451:U:H5''	1.96	0.48
45:CS:16:GLU:HG2	45:CS:100:GLY:HA2	1.95	0.48
53:DI:50:VAL:HG11	53:DI:92:ALA:HB2	1.94	0.48
54:DA:588:U:H2'	54:DA:589:U:C6	2.49	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:C1	2.44	0.48
1:BA:1493:A:H8	1:BA:1493:A:OP2	1.97	0.48
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.79	0.48
31:CA:323:C:H5'	32:CE:163:ASN:HD21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DS:92:TRP:CZ2	63:DS:201:PGE:H2	2.49	0.48
1:AA:451:A:H61	1:AA:481:G:H5'	1.79	0.48
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.94	0.48
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.44	0.48
31:CA:538:A:H4'	37:CK:7:LYS:HG2	1.96	0.48
31:CA:674:G:H2'	31:CA:804:A:H61	1.79	0.48
31:CA:796:C:H2'	31:CA:797:G:C8	2.49	0.48
54:DA:2031:A:C6	54:DA:2498:OMC:H1'	2.48	0.48
54:DA:2262:U:H4'	54:DA:2328:A:C2	2.49	0.48
54:DA:2262:U:H4'	54:DA:2328:A:H2	1.79	0.48
29:CC:228:VAL:HG21	69:CA:3410:HOH:O	2.13	0.47
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.47
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.49	0.47
35:CH:82:SER:HB2	35:CH:94:ILE:HD11	1.96	0.47
46:CT:86:MET:HE3	46:CT:87:PRO:HD2	1.95	0.47
48:DV:17:LYS:HE3	48:DV:40:ASN:HA	1.96	0.47
1:BA:1346:A:H61	1:BA:1374:A:H3'	1.78	0.47
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.95	0.47
41:CO:55:ALA:HA	41:CO:80:PHE:CE2	2.49	0.47
42:CP:35:ILE:HG21	42:CP:71:ALA:HA	1.96	0.47
54:DA:1433:A:O2'	54:DA:1434:A:H5'	2.14	0.47
20:AT:24:ARG:HD3	20:AT:24:ARG:N	2.30	0.47
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.96	0.47
34:CG:164:TYR:HB2	34:CG:167:GLU:HB2	1.95	0.47
38:CL:1:MET:HE3	38:CL:32:TYR:CZ	2.50	0.47
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.79	0.47
52:CZ:42:LEU:HD23	52:CZ:45:GLN:HE21	1.79	0.47
40:DN:33:LEU:HD13	40:DN:117:PHE:HB3	1.95	0.47
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.30	0.47
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.97	0.47
31:CA:804:A:H2'	31:CA:806:C:C4	2.49	0.47
53:DI:44:ALA:HB1	53:DI:95:LEU:HD11	1.96	0.47
1:AA:518:C:H2'	1:AA:530:G:C8	2.48	0.47
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.79	0.47
31:CA:588:U:H2'	31:CA:589:U:C6	2.49	0.47
31:CA:634:C:H2'	31:CA:635:C:C6	2.50	0.47
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.97	0.47
29:DC:3:VAL:HG21	29:DC:202:LEU:HD23	1.96	0.47
39:CM:85:VAL:HG11	39:CM:90:VAL:HG22	1.96	0.47
42:DP:9:ARG:HH22	54:DA:2295:C:P	2.38	0.47
44:DR:19:LYS:HD3	56:DR:202:PG4:H22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:2520:C:C6	54:DA:2567:G:H1'	2.50	0.47
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.47
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.96	0.47
3:BC:26:THR:HG23	14:BN:76:LYS:HD2	1.96	0.47
13:BM:77:ILE:HG22	13:BM:81:MET:HE2	1.96	0.47
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.95	0.47
24:D3:7:PRO:HB2	54:DA:1309:G:H4'	1.95	0.47
31:CA:70:G:H5''	31:CA:112:U:O2	2.14	0.47
31:CA:737:C:H42	31:CA:759:G:H1	1.63	0.47
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.15	0.47
31:CA:2686:G:H2'	31:CA:2687:U:C6	2.50	0.47
39:CM:19:LEU:HD23	39:CM:31:GLY:O	2.15	0.47
39:CM:28:GLY:O	39:CM:29:LYS:O	2.33	0.47
44:CR:87:SER:HB3	45:CS:52:PRO:HD3	1.96	0.47
49:CW:51:GLN:HG2	49:CW:86:LEU:HD11	1.97	0.47
54:DA:2324:U:H3'	54:DA:2325:G:H5''	1.97	0.47
1:AA:946:A:H2'	1:AA:947:G:C8	2.50	0.47
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.95	0.47
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.15	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.96	0.47
1:BA:214:C:H2'	1:BA:215:C:H6	1.80	0.47
1:BA:946:A:H2'	1:BA:947:G:C8	2.50	0.47
1:BA:957:U:O2	1:BA:959:A:H8	1.98	0.47
31:CA:248:G:H5'	31:CA:250:G:N7	2.29	0.47
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.80	0.47
40:CN:21:ALA:HB1	40:CN:100:LYS:HG2	1.97	0.47
48:CV:94:ARG:HB3	48:CV:103:ILE:HD12	1.97	0.47
54:DA:5:A:H2'	54:DA:6:A:C8	2.50	0.47
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.96	0.47
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.47
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.15	0.47
31:CA:1914:C:H2'	31:CA:1915:3TD:H6	1.96	0.47
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.50	0.47
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.47
41:CO:47:VAL:O	41:CO:51:LEU:HD23	2.15	0.47
39:DM:21:ARG:HA	54:DA:811:U:H2'	1.96	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.14	0.46
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.97	0.46
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.97	0.46
1:BA:1250:A:O3'	9:BI:69:GLY:HA2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46
31:CA:976:G:H2'	31:CA:977:G:H8	1.80	0.46
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.50	0.46
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.50	0.46
35:DH:82:SER:HB2	35:DH:94:ILE:HD11	1.95	0.46
54:DA:933:A:H5'	54:DA:934:U:OP2	2.14	0.46
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.54	0.46
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.46
31:CA:443:A:H2'	32:CE:40:ARG:NH1	2.29	0.46
39:CM:21:ARG:CG	39:CM:21:ARG:NH2	2.76	0.46
54:DA:1738:G:HO2'	54:DA:1739:A:H8	1.61	0.46
54:DA:2128:G:H1	54:DA:2160:C:N4	2.12	0.46
1:AA:429:U:H1'	1:AA:430:A:H5''	1.97	0.46
13:AM:77:ILE:HG22	13:AM:81:MET:HE2	1.96	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.98	0.46
42:CP:7:ARG:HA	42:CP:10:ARG:HE	1.79	0.46
33:DF:5:HIS:HD1	33:DF:97:TRP:NE1	2.13	0.46
19:AS:32:ARG:HE	19:AS:57:HIS:CE1	2.34	0.46
1:BA:411:A:P	4:BD:26:ARG:HH12	2.38	0.46
1:BA:429:U:H1'	1:BA:430:A:H5''	1.98	0.46
1:BA:1152:A:H2'	1:BA:1153:G:C8	2.51	0.46
31:CA:727:A:H2'	31:CA:728:G:C8	2.50	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.50	0.46
29:DC:207:LYS:HB2	54:DA:729:G:C6	2.50	0.46
7:AG:132:GLY:H	7:AG:135:VAL:HG22	1.80	0.46
31:CA:933:A:H5'	31:CA:934:U:OP2	2.16	0.46
31:CA:1386:C:H2'	31:CA:1387:A:C8	2.51	0.46
33:CF:5:HIS:HE2	33:CF:9:LYS:HE3	1.80	0.46
34:DG:52:PHE:CD1	34:DG:52:PHE:N	2.84	0.46
38:DL:101:GLY:O	38:DL:120:PRO:HD2	2.16	0.46
54:DA:265:A:H4'	54:DA:266:G:OP1	2.16	0.46
54:DA:2895:G:H2'	54:DA:2896:C:C6	2.51	0.46
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.97	0.46
12:AL:43:LYS:HE2	12:AL:89:D2T:H7	1.97	0.46
12:BL:110:ARG:NH2	12:BL:117:TYR:CE2	2.84	0.46
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.96	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.98	0.46
42:CP:51:ALA:HB3	42:CP:78:VAL:HG13	1.98	0.46
51:DY:10:LYS:HE3	51:DY:54:LYS:HG2	1.97	0.46
18:BR:41:PRO:HG2	18:BR:44:ILE:HD12	1.97	0.46
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	1.96	0.46
30:DD:121:THR:HB	30:DD:127:PHE:CD2	2.51	0.46
40:CN:33:LEU:HD13	40:CN:117:PHE:HB3	1.97	0.46
44:CR:22:LYS:HE2	44:CR:22:LYS:HA	1.97	0.46
49:DW:51:GLN:HG2	49:DW:86:LEU:HD11	1.98	0.46
54:DA:2243:U:H2'	54:DA:2244:U:C6	2.51	0.46
1:AA:76:G:H22	1:AA:93:U:H3	1.64	0.46
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.98	0.46
31:CA:686:U:H2'	31:CA:788:A:N1	2.31	0.46
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.98	0.46
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.51	0.46
45:CS:7:SER:HB3	45:CS:12:HIS:HE1	1.79	0.46
54:DA:1168:G:H2'	54:DA:1169:A:O4'	2.15	0.46
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.51	0.46
1:AA:1239:A:H62	1:AA:1299:A:N6	2.14	0.46
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.81	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
31:CA:493:G:H2'	31:CA:494:G:O4'	2.16	0.46
31:CA:2030:6MZ:C2	31:CA:2499:C:H5''	2.46	0.46
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.15	0.46
38:DL:76:VAL:CG2	54:DA:2684:U:H4'	2.46	0.46
54:DA:493:G:H2'	54:DA:494:G:O4'	2.16	0.46
54:DA:1738:G:O2'	54:DA:1739:A:H8	1.99	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.16	0.46
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.15	0.46
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.16	0.46
33:CF:31:VAL:HG11	33:CF:97:TRP:CH2	2.51	0.46
50:DX:11:ARG:HH11	54:DA:2256:G:H4'	1.81	0.46
1:AA:957:U:O2	1:AA:959:A:H8	1.98	0.45
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.82	0.45
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.51	0.45
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.80	0.45
1:BA:439:U:H5''	4:BD:121:LYS:HD2	1.97	0.45
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.97	0.45
40:DN:75:GLU:HB2	40:DN:90:GLU:HG3	1.97	0.45
54:DA:68:G:H2'	54:DA:69:C:O4'	2.16	0.45
54:DA:1510:G:H2'	54:DA:1511:G:O4'	2.16	0.45
54:DA:2133:G:H21	54:DA:2158:A:N6	2.14	0.45
3:AC:26:THR:HG23	14:AN:76:LYS:HD2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:15:LEU:HA	5:AE:37:THR:HG22	1.98	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.97	0.45
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.15	0.45
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.98	0.45
38:CL:7:MET:HE1	38:CL:44:LYS:HG3	1.98	0.45
51:CY:10:LYS:HE3	51:CY:54:LYS:HG2	1.96	0.45
50:DX:39:ARG:HD3	69:DX:118:HOH:O	2.16	0.45
54:DA:722:A:H2'	54:DA:723:C:O4'	2.16	0.45
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.98	0.45
5:BE:15:LEU:HA	5:BE:37:THR:HG22	1.98	0.45
31:CA:998:C:OP2	44:CR:58:ARG:NH2	2.49	0.45
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.81	0.45
31:CA:2895:G:H2'	31:CA:2896:C:C6	2.51	0.45
54:DA:2547:A:H2'	54:DA:2548:U:C6	2.52	0.45
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.97	0.45
1:BA:76:G:H22	1:BA:93:U:H3	1.64	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.17	0.45
31:CA:969:G:H2'	31:CA:970:U:C6	2.52	0.45
54:DA:1386:C:H2'	54:DA:1387:A:C8	2.51	0.45
54:DA:2328:A:H2'	54:DA:2329:U:C6	2.51	0.45
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HA	1.99	0.45
31:CA:1936:A:N6	31:CA:1963:U:H3	2.14	0.45
30:DD:150[B]:MEQ:HE2	54:DA:2033:A:O5'	2.16	0.45
54:DA:686:U:H2'	54:DA:788:A:N1	2.31	0.45
54:DA:788:A:H5''	58:DA:3222:PUT:H12	1.99	0.45
12:AL:110:ARG:NH2	12:AL:117:TYR:CE2	2.85	0.45
18:AR:41:PRO:HG2	18:AR:44:ILE:HD12	1.98	0.45
1:BA:451:A:H61	1:BA:481:G:H5'	1.81	0.45
1:BA:545:C:H5'	4:BD:69:GLU:HB2	1.98	0.45
1:BA:1239:A:H62	1:BA:1299:A:N6	2.14	0.45
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.97	0.45
20:BT:48:GLN:HE21	20:BT:83:ILE:HD13	1.81	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
38:CL:101:GLY:O	38:CL:120:PRO:HD2	2.15	0.45
1:AA:604:G:H2'	1:AA:605:U:O4'	2.17	0.45
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.51	0.45
1:BA:328:C:H2'	1:BA:328:C:O2	2.17	0.45
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.97	0.45
30:CD:129:THR:CG2	30:CD:140:HIS:O	2.65	0.45
31:CA:1936:A:C2	31:CA:1943:U:N3	2.61	0.45
44:DR:34:VAL:HG21	54:DA:2019:A:H4'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:747:5MU:O2	54:DA:2014:A:H1'	2.17	0.45
54:DA:788:A:H3'	58:DA:3222:PUT:H41	1.98	0.45
54:DA:1494:A:H2'	54:DA:1495:A:C8	2.51	0.45
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.45
1:AA:1239:A:H62	1:AA:1299:A:H62	1.64	0.45
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.99	0.45
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.82	0.45
5:BE:76:LEU:HD21	5:BE:120:VAL:HG22	1.99	0.45
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.98	0.45
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.32	0.45
48:CV:45:HIS:CD2	48:CV:58:ILE:HG12	2.50	0.45
33:DF:121:SER:HB2	54:DA:2304:G:H5'	1.98	0.45
42:DP:51:ALA:HB3	42:DP:78:VAL:HG13	1.99	0.45
54:DA:136:G:H1	54:DA:143:C:N4	2.15	0.45
1:AA:528:C:H5''	1:AA:528:C:C6	2.52	0.45
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.45
7:BG:132:GLY:H	7:BG:135:VAL:HG22	1.81	0.45
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.45
40:DN:14:LYS:HE2	69:DA:3581:HOH:O	2.16	0.45
1:AA:1068:G:N7	1:AA:1094:G:H2'	2.32	0.45
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.82	0.45
1:BA:604:G:H2'	1:BA:605:U:O4'	2.17	0.45
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.81	0.45
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.98	0.45
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.17	0.45
54:DA:278:A:N3	54:DA:278:A:H2'	2.32	0.45
54:DA:825:A:H2'	54:DA:826:U:O4'	2.17	0.45
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.52	0.45
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	1.99	0.44
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	1.98	0.44
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	1.99	0.44
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.81	0.44
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.99	0.44
17:BQ:51:ASN:N	17:BQ:51:ASN:HD22	2.15	0.44
22:D1:25:VAL:HG11	46:DT:38:TYR:HB2	1.99	0.44
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.30	0.44
31:CA:1327:A:H2'	31:CA:1328:A:O4'	2.17	0.44
54:DA:639:U:H2'	54:DA:640:C:C6	2.52	0.44
1:AA:545:C:H5'	4:AD:69:GLU:HB2	1.98	0.44
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.54	0.44
31:CA:1214:A:H4'	31:CA:1239:G:H4'	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1101:U:H2'	54:DA:1102:C:C6	2.52	0.44
1:AA:79:G:H22	1:AA:90:C:H42	1.66	0.44
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.98	0.44
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.00	0.44
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.81	0.44
23:D2:15:ALA:HB2	23:D2:47:VAL:HG21	1.99	0.44
32:CE:72:SER:C	32:CE:74:LYS:H	2.25	0.44
44:CR:58:ARG:NH1	44:CR:62:ILE:HD11	2.32	0.44
54:DA:455:C:N3	54:DA:472:A:H2'	2.31	0.44
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.98	0.44
1:BA:134:G:H2'	1:BA:135:C:O4'	2.18	0.44
1:BA:1069:C:O4'	1:BA:1191:A:H2	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.52	0.44
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.99	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.31	0.44
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.33	0.44
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.53	0.44
38:DL:7:MET:HE1	38:DL:44:LYS:HG3	1.99	0.44
40:DN:41:LEU:CD2	40:DN:125:PRO:HD2	2.47	0.44
54:DA:2722:G:H2'	54:DA:2723:C:C6	2.53	0.44
54:DA:2747:G:O6	54:DA:2755:C:H5''	2.17	0.44
1:AA:345:C:H5''	43:DQ:34:GLU:O	2.17	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:N	2.33	0.44
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.99	0.44
14:AN:89:MET:HE1	14:AN:98:LYS:HD2	2.00	0.44
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.54	0.44
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.82	0.44
31:CA:136:G:H1	31:CA:143:C:N4	2.16	0.44
34:CG:52:PHE:CD2	34:CG:52:PHE:N	2.86	0.44
40:CN:75:GLU:HB2	40:CN:90:GLU:HG3	2.00	0.44
35:DH:1:MET:HE3	35:DH:23:ALA:HA	1.99	0.44
50:DX:11:ARG:H	50:DX:11:ARG:HE	1.65	0.44
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.32	0.44
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.53	0.44
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.99	0.44
29:CC:219:THR:O	31:CA:1789:A:H5''	2.17	0.44
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.17	0.44
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.83	0.44
41:CO:28:LEU:HD23	41:CO:48:VAL:HG21	1.99	0.44
39:DM:85:VAL:HB	39:DM:94:THR:HG22	1.99	0.44
45:DS:21:ARG:HH21	56:DS:202:PG4:H71	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1637:A:H5'	54:DA:1760:C:O2'	2.17	0.44
54:DA:2723:C:O5'	54:DA:2723:C:H6	2.01	0.44
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.82	0.44
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.99	0.44
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.16	0.44
7:BG:69:VAL:HG21	7:BG:104:ILE:HD11	1.99	0.44
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.53	0.44
31:CA:17:G:H4'	44:CR:25:TYR:HE2	1.81	0.44
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.52	0.44
31:CA:2298:A:C2	31:CA:2321:U:N3	2.85	0.44
31:CA:2394:C:H5''	39:CM:63:LYS:HE2	2.00	0.44
30:DD:55:LYS:HD3	30:DD:60:VAL:HG22	2.00	0.44
35:CH:104:THR:HG22	35:CH:109:GLU:HA	2.00	0.44
53:DI:50:VAL:HG22	53:DI:85:VAL:HG13	1.99	0.44
54:DA:2117:A:H61	54:DA:2171:A:H61	1.66	0.44
21:BU:51:SER:HA	21:BU:54:LYS:HE3	2.00	0.44
31:CA:142:A:H1'	47:CU:1:MET:HB3	1.99	0.44
31:CA:671:C:C5	39:CM:33:ARG:NH2	2.86	0.44
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.52	0.44
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.52	0.44
40:CN:42:THR:HA	40:CN:93:VAL:HG12	2.00	0.44
35:DH:104:THR:HG22	35:DH:109:GLU:HA	1.99	0.44
54:DA:2473:U:O2	54:DA:2473:U:H2'	2.18	0.44
1:AA:240:G:H4'	1:AA:240:G:OP1	2.17	0.44
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.44
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.17	0.44
1:BA:677:U:H3	1:BA:713:G:H22	1.66	0.44
1:BA:1432:G:H3'	43:CQ:106:LYS:HE2	1.99	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.52	0.44
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.17	0.44
47:DU:33:LYS:HG3	47:DU:80:TRP:CE3	2.52	0.44
54:DA:352:A:H5''	54:DA:352:A:H8	1.82	0.44
1:AA:1152:A:H2'	1:AA:1153:G:C8	2.53	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.00	0.43
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.18	0.43
1:BA:1239:A:H62	1:BA:1299:A:H62	1.64	0.43
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.83	0.43
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.83	0.43
48:DV:66:GLN:HG3	54:DA:328:U:O3'	2.17	0.43
54:DA:142:A:H2'	54:DA:143:C:C6	2.52	0.43
54:DA:207:A:H2'	54:DA:208:C:O4'	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1180:U:H5''	54:DA:1180:U:C6	2.52	0.43
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.83	0.43
1:BA:774:G:H21	56:BA:1642:PG4:H62	1.84	0.43
30:DD:25:THR:HG21	30:DD:193:VAL:HG22	2.00	0.43
38:CL:105:ARG:HH21	43:CQ:34:GLU:HG2	1.84	0.43
47:CU:33:LYS:HG3	47:CU:80:TRP:CE3	2.53	0.43
40:DN:42:THR:HG22	40:DN:93:VAL:HG12	1.99	0.43
42:DP:27:VAL:HG21	42:DP:40:ILE:HD12	2.00	0.43
44:DR:19:LYS:HB3	56:DR:202:PG4:H41	2.00	0.43
54:DA:31:C:O3'	54:DA:1238:G:H5''	2.17	0.43
1:BA:844:G:H2'	1:BA:844:G:N3	2.32	0.43
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.99	0.43
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.99	0.43
35:CH:78:VAL:HG21	35:CH:103:VAL:HG22	2.00	0.43
49:DW:51:GLN:HB2	49:DW:57:TYR:OH	2.18	0.43
54:DA:553:G:H2'	54:DA:554:U:O4'	2.18	0.43
1:AA:1358:U:H3	1:AA:1363:A:H62	1.66	0.43
1:BA:1329:A:H5''	13:BM:26:GLY:N	2.33	0.43
31:CA:2473:U:O2	31:CA:2473:U:H2'	2.18	0.43
1:AA:202:G:H21	1:AA:466:A:H61	1.65	0.43
27:C0:2:ALA:CB	27:C0:39:GLU:HB3	2.49	0.43
1:BA:1152:A:H2'	1:BA:1153:G:H8	1.82	0.43
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.18	0.43
28:CB:57:A:C4'	33:CF:27:GLN:HG3	2.49	0.43
28:CB:57:A:O4'	33:CF:27:GLN:HG3	2.17	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
31:CA:265:A:H4'	31:CA:266:G:OP1	2.19	0.43
31:CA:2114:A:N6	31:CA:2119:A:H62	2.16	0.43
32:DE:45:ALA:HB3	54:DA:38:A:H5'	2.01	0.43
40:DN:40:ARG:HD3	40:DN:93:VAL:HG21	2.00	0.43
53:DI:94:ARG:HG2	53:DI:127:ALA:HA	2.01	0.43
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.18	0.43
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	2.00	0.43
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	2.01	0.43
1:BA:8:A:H5'	5:BE:125:ALA:O	2.18	0.43
1:BA:322:C:H5	1:BA:328:C:C5	2.36	0.43
13:BM:23:TYR:HD1	13:BM:69:LEU:HD23	1.84	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.48	0.43
31:CA:459:U:C5	31:CA:469:G:N2	2.87	0.43
31:CA:871:U:H2'	31:CA:872:U:C6	2.53	0.43
30:DD:150[B]:MEQ:HG3	54:DA:2032:G:N3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CF:103:LEU:HA	33:CF:107:ALA:HB3	2.01	0.43
54:DA:26:G:H1'	54:DA:514:A:N6	2.33	0.43
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.54	0.43
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	2.00	0.43
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.54	0.43
31:CA:532:A:N1	31:CA:2020:A:H1'	2.34	0.43
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.54	0.43
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.53	0.43
54:DA:984:A:N3	54:DA:984:A:H2'	2.33	0.43
54:DA:1778:U:H2'	54:DA:1784:A:N6	2.34	0.43
1:AA:216:U:H2'	1:AA:217:C:C6	2.53	0.43
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.59	0.43
5:BE:88:VAL:CG1	5:BE:93:ARG:HG2	2.48	0.43
14:BN:89:MET:HE1	14:BN:98:LYS:HD2	2.01	0.43
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	2.01	0.43
31:CA:321:U:H5''	32:CE:131:THR:HG23	2.01	0.43
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	2.00	0.43
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.84	0.43
33:DF:103:LEU:HA	33:DF:107:ALA:HB3	2.00	0.43
54:DA:1469:A:H2'	54:DA:1470:A:C8	2.54	0.43
54:DA:1587:G:H2'	54:DA:1588:G:H8	1.84	0.43
54:DA:2233:U:H2'	54:DA:2234:G:C8	2.54	0.43
1:AA:567:G:H2'	1:AA:568:G:O4'	2.19	0.43
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	2.00	0.43
31:CA:1028:A:H61	31:CA:1125:G:H2'	1.84	0.43
32:CE:75:SER:O	32:CE:78:TRP:HB2	2.18	0.43
49:CW:77:VAL:HG23	49:CW:89:ILE:HG12	2.00	0.43
36:DJ:19:ASN:N	36:DJ:20:PRO:HD2	2.33	0.43
54:DA:644:A:H2'	54:DA:645:C:O4'	2.19	0.43
54:DA:2097:A:H8	54:DA:2097:A:H5''	1.84	0.43
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.19	0.43
25:C4:62:LEU:HB3	25:C4:65:ALA:HB2	2.01	0.43
1:BA:8:A:H1'	5:BE:108:GLY:HA2	2.00	0.43
1:BA:663:A:H5'	1:BA:836:G:OP1	2.19	0.43
29:CC:258:ARG:NH1	29:CC:264:ASP:OD1	2.52	0.43
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.84	0.43
31:CA:1427:A:H4'	31:CA:1428:C:O4'	2.18	0.43
31:CA:1662:U:H3	31:CA:1998:A:H61	1.66	0.43
33:CF:36:LEU:HD12	33:CF:154:ILE:HG12	2.01	0.43
43:DQ:6:LYS:O	43:DQ:10:GLN:HG2	2.19	0.43
47:DU:28:ASN:OD1	47:DU:91:GLN:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.53	0.42
4:BD:28:ILE:HG12	4:BD:34:ILE:HD13	2.01	0.42
29:CC:69:ARG:HB2	29:CC:129:THR:HG21	2.00	0.42
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.99	0.42
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	2.00	0.42
34:CG:19:ILE:HG12	34:CG:24:ILE:HG12	2.01	0.42
52:CZ:46:VAL:O	52:CZ:50:VAL:HG23	2.19	0.42
50:DX:41[B]:ARG:HA	50:DX:41[B]:ARG:HD3	1.77	0.42
51:DY:57:ARG:NH1	54:DA:400:G:N7	2.55	0.42
1:AA:268:U:H2'	1:AA:269:C:C6	2.54	0.42
1:AA:1081:A:H5'	5:AE:23:LYS:HG3	2.00	0.42
1:AA:1366:C:H2'	1:AA:1367:C:C6	2.54	0.42
5:AE:81:LEU:HB3	5:AE:147:MET:SD	2.59	0.42
13:AM:80:LEU:HD22	13:AM:87:ARG:HB3	2.02	0.42
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.54	0.42
25:D4:13:ARG:HG3	39:DM:63:LYS:HA	2.01	0.42
28:CB:14:U:H2'	28:CB:15:A:C2	2.53	0.42
31:CA:352:A:H8	31:CA:352:A:H5''	1.84	0.42
31:CA:2543:G:H2'	31:CA:2544:G:C8	2.55	0.42
39:CM:77:ILE:HD11	39:CM:108:ALA:CB	2.35	0.42
45:CS:16:GLU:HG3	45:CS:101:ILE:HG12	1.99	0.42
51:DY:7:VAL:HG23	51:DY:51:VAL:HG12	2.00	0.42
54:DA:476:G:H4'	54:DA:502:A:N1	2.34	0.42
54:DA:1026:G:H2'	54:DA:1027:A:C8	2.54	0.42
4:AD:28:ILE:HG12	4:AD:34:ILE:HD13	2.01	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.85	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.01	0.42
31:CA:1937:A:H1'	31:CA:1939:5MU:H72	2.02	0.42
30:DD:35:THR:HG22	30:DD:73:VAL:HG21	2.01	0.42
35:CH:3:VAL:HG12	35:CH:38:PRO:HA	2.00	0.42
45:CS:37:GLU:HB3	45:CS:53:PHE:CD1	2.54	0.42
32:DE:94:GLN:HG2	54:DA:660:C:H5''	2.02	0.42
41:DO:28:LEU:HD23	41:DO:48:VAL:HG21	2.00	0.42
54:DA:2051:A:H8	54:DA:2051:A:OP2	2.02	0.42
1:AA:134:G:H2'	1:AA:135:C:O4'	2.19	0.42
1:AA:663:A:H5'	1:AA:836:G:OP1	2.19	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.02	0.42
9:BI:98:LEU:HB3	9:BI:104:VAL:HG13	2.01	0.42
31:CA:123:G:H4'	31:CA:1376:C:O5'	2.20	0.42
31:CA:948:C:H1'	31:CA:984:A:C8	2.54	0.42
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CK:58:ASN:HA	37:CK:126:ALA:O	2.19	0.42
54:DA:2813:A:H2	54:DA:2887[B]:A:N6	2.17	0.42
1:AA:967:5MC:O3'	9:AI:127:PHE:HE1	2.03	0.42
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	2.01	0.42
29:CC:208:ALA:CB	31:CA:1790:C:H4'	2.50	0.42
31:CA:478:A:H61	31:CA:500:G:H4'	1.84	0.42
31:CA:2579:C:H2'	31:CA:2580:PSU:O4'	2.19	0.42
47:CU:45:ALA:O	47:CU:49:LYS:HG2	2.19	0.42
49:CW:38:LEU:HD21	49:CW:65:VAL:HG11	2.01	0.42
50:CX:18:ALA:HB3	50:CX:20:ARG:NH1	2.33	0.42
53:DI:130:PRO:HG2	53:DI:134:GLU:HG2	2.01	0.42
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.18	0.42
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	2.02	0.42
11:BK:34:ILE:HB	11:BK:74:VAL:HG11	2.01	0.42
30:CD:55:LYS:HD3	30:CD:60:VAL:HG22	2.02	0.42
30:CD:101:PHE:O	30:CD:104:VAL:HG22	2.19	0.42
30:CD:186:LEU:HD21	43:CQ:4:ILE:HG21	2.01	0.42
31:CA:121:G:H4'	31:CA:149:A:H5'	2.02	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.55	0.42
31:CA:1005:C:HO2'	37:CK:30:THR:HG21	1.76	0.42
43:CQ:6:LYS:O	43:CQ:10:GLN:HG2	2.20	0.42
34:DG:19:ILE:HG12	34:DG:24:ILE:HG12	2.00	0.42
54:DA:191:A:H2'	54:DA:192:C:C6	2.55	0.42
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	2.02	0.42
1:BA:1338:G:H2'	1:BA:1339:A:C8	2.54	0.42
16:BP:6:LEU:HD23	16:BP:19:VAL:HB	2.00	0.42
31:CA:659:G:H4'	32:CE:95:LYS:HD3	2.02	0.42
31:CA:732:C:H2'	31:CA:733:G:O4'	2.20	0.42
31:CA:785:G:H4'	31:CA:1779:U:H4'	2.00	0.42
31:CA:1539:U:H2'	31:CA:1540:G:C8	2.55	0.42
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.20	0.42
29:DC:69:ARG:HB2	29:DC:129:THR:HG21	2.01	0.42
35:DH:116:ARG:HH21	35:DH:133:GLN:HB2	1.85	0.42
53:DI:26:VAL:HB	53:DI:83:ALA:HB3	2.00	0.42
54:DA:1168:G:H8	54:DA:1168:G:H5''	1.84	0.42
1:AA:1171:A:H2'	1:AA:1172:C:C6	2.54	0.42
27:C0:6:LYS:HB2	27:C0:58:GLU:HG3	2.02	0.42
1:BA:216:U:H2'	1:BA:217:C:C6	2.54	0.42
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.19	0.42
23:D2:6:ARG:HG2	23:D2:24:THR:HB	2.02	0.42
31:CA:191:A:H2'	31:CA:192:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:528:A:H8	31:CA:528:A:H3'	1.84	0.42
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.55	0.42
42:CP:27:VAL:HG21	42:CP:40:ILE:HD12	2.00	0.42
54:DA:1236:G:N7	58:DA:3189:PUT:H41	2.35	0.42
6:AF:9:MET:HG2	6:AF:86:ARG:HB3	2.01	0.42
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.01	0.42
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.01	0.42
1:BA:73:C:O2'	1:BA:74:A:H8	2.03	0.42
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.02	0.42
13:BM:23:TYR:CD1	13:BM:69:LEU:HD23	2.55	0.42
31:CA:246:C:O2'	31:CA:385:C:H4'	2.20	0.42
35:DH:78:VAL:HG21	35:DH:103:VAL:HG22	2.02	0.42
45:DS:16:GLU:HG3	45:DS:101:ILE:HG12	2.02	0.42
49:DW:38:LEU:HD21	49:DW:65:VAL:HG11	2.01	0.42
54:DA:1424:G:H21	63:DA:3214:PGE:H32	1.84	0.42
1:AA:932:C:H5'	7:AG:4:ARG:HE	1.84	0.42
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.42
1:BA:1308:U:H2'	1:BA:1309:G:H8	1.85	0.42
31:CA:834:G:H1'	31:CA:2358:A:N3	2.35	0.42
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.20	0.42
39:DM:57:LEU:HA	39:DM:60:ARG:HG3	2.02	0.42
44:DR:6:ARG:HD3	54:DA:1250:G:H5''	2.02	0.42
51:DY:51:VAL:HG23	51:DY:56:MET:HE2	2.02	0.42
54:DA:357:C:H2'	54:DA:358:U:C6	2.55	0.42
54:DA:2479:U:OP1	54:DA:2537:U:H1'	2.20	0.42
1:AA:49:U:O2	1:AA:362:G:H1'	2.20	0.41
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.41
1:AA:1396:A:H3'	59:AA:1681:TAC:C43	2.48	0.41
23:C2:6:ARG:HG2	23:C2:24:THR:HB	2.01	0.41
24:C3:19:ARG:HD3	31:CA:125:A:OP2	2.20	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.19	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.18	0.41
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.35	0.41
1:BA:1366:C:H2'	1:BA:1367:C:C6	2.55	0.41
30:CD:155:VAL:HG11	30:CD:161:MET:CE	2.50	0.41
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.55	0.41
32:CE:49:ARG:O	32:CE:74:LYS:HD2	2.20	0.41
32:CE:149:ILE:HG23	32:CE:188:MET:HG2	2.02	0.41
36:CJ:11:LEU:HD22	36:CJ:24:VAL:HG23	2.02	0.41
44:CR:113:ALA:O	44:CR:117:LEU:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DK:58:ASN:HA	37:DK:126:ALA:O	2.20	0.41
40:DN:92:TRP:HE1	57:DN:201:MPD:HM1	1.83	0.41
42:DP:41:ALA:HB2	42:DP:48:LEU:HD21	2.01	0.41
44:DR:20:GLN:HG3	56:DR:202:PG4:C4	2.40	0.41
46:DT:86:MET:HE3	46:DT:87:PRO:HD2	2.02	0.41
54:DA:527:C:H4'	54:DA:528:A:O5'	2.19	0.41
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	2.01	0.41
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	2.03	0.41
1:BA:716:A:N3	11:BK:119:ASN:O	2.53	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.50	0.41
17:BQ:47:HIS:HB2	17:BQ:67:LEU:HD13	2.01	0.41
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.55	0.41
31:CA:2544:G:H2'	31:CA:2545:G:O4'	2.20	0.41
29:DC:220:VAL:HG21	54:DA:782:A:N7	2.36	0.41
36:DJ:11:LEU:HD22	36:DJ:24:VAL:HG23	2.03	0.41
45:DS:86:GLN:HG2	69:DS:318:HOH:O	2.20	0.41
54:DA:264:C:O2'	54:DA:265:A:H2'	2.20	0.41
54:DA:871:U:H2'	54:DA:872:U:C6	2.55	0.41
1:BA:268:U:H2'	1:BA:269:C:C6	2.55	0.41
19:BS:33:THR:HG22	19:BS:35:SER:H	1.86	0.41
31:CA:826:U:O2'	39:CM:53:GLY:HA3	2.19	0.41
44:CR:76:TYR:CZ	44:CR:80:ILE:HG13	2.55	0.41
51:CY:12:PRO:HB3	51:CY:30:LEU:HD23	2.02	0.41
34:DG:26:ILE:O	34:DG:79:VAL:HG11	2.20	0.41
1:AA:77:A:H2'	1:AA:78:A:C8	2.56	0.41
1:AA:307:C:C4	57:AA:1676:MPD:H12	2.52	0.41
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.03	0.41
1:AA:716:A:N3	11:AK:119:ASN:O	2.53	0.41
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.35	0.41
1:BA:79:G:H22	1:BA:90:C:H42	1.67	0.41
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.21	0.41
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.19	0.41
5:BE:149:SER:HB2	5:BE:151:GLU:HG2	2.02	0.41
29:DC:97:LYS:HA	29:DC:97:LYS:HD3	1.72	0.41
29:DC:231:PRO:C	29:DC:233:GLY:H	2.28	0.41
39:CM:95:LEU:HD22	39:CM:100:ILE:HG12	2.02	0.41
35:DH:71:LYS:HB3	35:DH:108:VAL:HG22	2.02	0.41
52:DZ:46:VAL:O	52:DZ:50:VAL:HG23	2.19	0.41
54:DA:2063:C:O2	54:DA:2450:A:N1	2.53	0.41
12:AL:36:ARG:HH11	12:AL:54:ARG:NH1	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:511:U:H5''	31:CA:1235:G:H4'	2.03	0.41
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	2.01	0.41
49:CW:51:GLN:HB2	49:CW:57:TYR:OH	2.21	0.41
33:DF:34:ILE:HG12	33:DF:156:ILE:HG12	2.02	0.41
34:DG:24:ILE:HG21	34:DG:72:LEU:HD21	2.02	0.41
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.01	0.41
1:AA:649:A:H2'	1:AA:650:G:O4'	2.20	0.41
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.56	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
1:BA:269:C:H2'	1:BA:270:A:C8	2.56	0.41
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.56	0.41
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.21	0.41
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	2.03	0.41
22:D1:25:VAL:HG11	46:DT:38:TYR:CB	2.51	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
31:CA:264:C:O2'	31:CA:265:A:H2'	2.20	0.41
31:CA:594:U:H2'	31:CA:595:C:C6	2.55	0.41
31:CA:729:G:H2'	31:CA:1775:U:H1'	2.02	0.41
31:CA:783:A:H2	31:CA:1778:U:H4'	1.85	0.41
31:CA:1154:G:OP1	44:CR:58:ARG:HD3	2.20	0.41
39:CM:79:LEU:O	39:CM:82:LEU:HG	2.21	0.41
35:DH:3:VAL:HG12	35:DH:38:PRO:HA	2.03	0.41
42:DP:53:THR:HB	42:DP:65:THR:HG22	2.02	0.41
54:DA:1539:U:H2'	54:DA:1540:G:C8	2.55	0.41
54:DA:2698:U:H2'	54:DA:2699:C:C6	2.56	0.41
1:AA:1152:A:H2'	1:AA:1153:G:H8	1.85	0.41
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.85	0.41
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.85	0.41
1:BA:310:G:H5''	16:BP:31:ARG:HB2	2.02	0.41
1:BA:591:U:H2'	1:BA:592:G:C8	2.55	0.41
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.56	0.41
10:BJ:80:THR:HG22	10:BJ:82:LYS:H	1.86	0.41
27:D0:8:THR:O	27:D0:55:VAL:HA	2.21	0.41
54:DA:121:G:H4'	54:DA:149:A:H5'	2.02	0.41
1:BA:629:A:H2'	1:BA:630:A:O4'	2.21	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.02	0.41
13:BM:80:LEU:HD22	13:BM:87:ARG:HB3	2.03	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.56	0.41
31:CA:563:A:H1'	31:CA:2018:G:N2	2.36	0.41
31:CA:845:A:H61	31:CA:932:U:H3	1.68	0.41
31:CA:1779:U:C5	31:CA:1784:A:N7	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DQ:25:THR:HB	43:DQ:88:ARG:HB3	2.03	0.41
54:DA:1720:U:H2'	54:DA:1721:G:O4'	2.20	0.41
54:DA:2070:A:H2'	54:DA:2071:A:O4'	2.21	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.55	0.41
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.20	0.41
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.03	0.41
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.03	0.41
1:BA:202:G:H21	1:BA:466:A:H61	1.67	0.41
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.02	0.41
29:CC:200:HIS:O	29:CC:203:ARG:HG2	2.21	0.41
31:CA:357:C:H2'	31:CA:358:U:C6	2.55	0.41
31:CA:388:G:N7	31:CA:390:U:H2'	2.35	0.41
31:CA:396:G:C1'	51:CY:29:PHE:HB3	2.49	0.41
31:CA:797:G:H5''	32:CE:55:SER:HB2	2.02	0.41
31:CA:2063:C:O2	31:CA:2450:A:N1	2.54	0.41
40:CN:71:LYS:HB3	40:CN:93:VAL:O	2.20	0.41
32:DE:32:VAL:HG21	39:DM:6:LEU:HD13	2.03	0.41
32:DE:49:ARG:O	32:DE:74:LYS:HD2	2.21	0.41
49:DW:77:VAL:HG23	49:DW:89:ILE:HG12	2.03	0.41
54:DA:2123:G:H2'	54:DA:2124:G:H8	1.85	0.41
54:DA:2813:A:H2	54:DA:2887[B]:A:H61	1.66	0.41
57:DA:3207:MPD:H11	57:DA:3207:MPD:H4	1.99	0.41
1:AA:9:G:H5'	5:AE:108:GLY:HA3	2.03	0.41
1:AA:269:C:H2'	1:AA:270:A:C8	2.55	0.41
1:AA:677:U:H3	1:AA:713:G:H22	1.69	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.41
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.54	0.41
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	2.03	0.41
16:BP:40:ASN:O	16:BP:43:ALA:HB2	2.21	0.41
49:CW:63:ILE:CD1	49:CW:72:VAL:HG21	2.50	0.41
45:DS:21:ARG:HH21	56:DS:202:PG4:C7	2.34	0.41
46:DT:17:VAL:HB	46:DT:76:VAL:HG11	2.03	0.41
46:DT:77:ASP:HB3	54:DA:24:G:O2'	2.20	0.41
54:DA:2336:A:N3	54:DA:2385:C:H1'	2.36	0.41
1:AA:629:A:H2'	1:AA:630:A:O4'	2.21	0.40
31:CA:225:C:H2'	31:CA:226:A:O4'	2.21	0.40
31:CA:372:G:H5''	51:CY:61:LYS:HD3	2.03	0.40
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.56	0.40
31:CA:1662:U:O2'	31:CA:2687:U:H5''	2.21	0.40
30:DD:167:ASN:HD21	62:DA:3198:EDO:H11	1.86	0.40
42:DP:103:VAL:HG23	69:DB:307:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:322:C:H5	1:AA:328:C:C5	2.38	0.40
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.56	0.40
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.56	0.40
26:D5:2:LYS:HE2	26:D5:4:ARG:HH11	1.86	0.40
30:CD:63:PRO:HG3	31:CA:2787:C:H1'	2.02	0.40
31:CA:2698:U:H2'	31:CA:2699:C:C6	2.56	0.40
32:CE:108:ILE:HG21	32:CE:181:ILE:HD11	2.04	0.40
54:DA:78:U:H2'	54:DA:79:C:C6	2.57	0.40
54:DA:1093:G:H1'	54:DA:1099:G:N2	2.37	0.40
54:DA:1354:A:H2'	54:DA:1355:G:O4'	2.21	0.40
54:DA:2678:C:H2'	54:DA:2679:A:O4'	2.20	0.40
1:AA:244:U:O4	1:AA:906:A:H1'	2.22	0.40
1:AA:920:U:H2'	1:AA:921:U:C6	2.57	0.40
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.56	0.40
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.40
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.04	0.40
22:D1:24:ALA:HB1	46:DT:35:ILE:HG12	2.03	0.40
29:CC:13:ARG:HD3	31:CA:728:G:H4'	2.03	0.40
31:CA:1808:A:N1	51:CY:28:ARG:HD2	2.36	0.40
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.22	0.40
35:CH:71:LYS:HB3	35:CH:108:VAL:HG22	2.04	0.40
44:DR:76:TYR:CZ	44:DR:80:ILE:HG13	2.56	0.40
47:DU:33:LYS:HE2	63:DU:101:PGE:C2	2.52	0.40
47:DU:33:LYS:NZ	63:DU:101:PGE:H62	2.36	0.40
47:DU:69:ARG:HG3	47:DU:74:ILE:HG22	2.03	0.40
50:DX:11:ARG:HG2	56:DA:3193:PG4:H12	2.04	0.40
54:DA:909:A:O2'	54:DA:910:A:H5'	2.21	0.40
54:DA:2022:U:H1'	69:DA:3881:HOH:O	2.21	0.40
54:DA:2545:G:N3	54:DA:2565:A:H2	2.20	0.40
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.02	0.40
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	2.04	0.40
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	2.02	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.86	0.40
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	2.02	0.40
1:BA:649:A:H2'	1:BA:650:G:O4'	2.21	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.37	0.40
31:CA:78:U:H2'	31:CA:79:C:C6	2.57	0.40
31:CA:586:A:H5'	32:CE:84:THR:HG21	2.02	0.40
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.57	0.40
31:CA:2305:U:H5''	33:CF:131:GLY:HA3	2.04	0.40
46:CT:17:VAL:HB	46:CT:76:VAL:HG11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DL:78:ARG:HD3	69:DL:308:HOH:O	2.21	0.40
54:DA:340:A:H2'	54:DA:341:C:O4'	2.22	0.40
63:DA:3001:PGE:H52	69:DA:5960:HOH:O	2.22	0.40
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.37	0.40
33:DF:14:LYS:O	33:DF:18:THR:HG22	2.21	0.40
37:DK:7:LYS:HG2	54:DA:538:A:H4'	2.03	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.04	0.40
51:DY:56:MET:HE1	54:DA:2091:C:O2'	2.22	0.40
54:DA:364:C:H2'	54:DA:365:U:C6	2.57	0.40
54:DA:2324:U:H3'	54:DA:2325:G:C5'	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	6	31
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	6	31
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	24	60
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	8	35
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	24	60
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	24	60
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	18	53
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	2	13
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	2	13
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	18	53
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	18	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	50
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	7	34
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	5	27
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1	6
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14	48
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	14	48
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16	50
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	4	22
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	12
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	6	28
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	12	45
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	40
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	38
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	23
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	9	38
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	10
18	AR	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	9	38
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	10	40
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	4	24
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1	8
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	25
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	7	34
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	7	34
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	21
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	2	16
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	8	35
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	18	53
30	CD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
30	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
32	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	8	35
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	24	60
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	21	56
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	11	43
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	5	25
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	21	56
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3	17
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	36
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	9	36
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	18	53
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7	32
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	7	32
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	27
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	53
40	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
40	DN	134/136 (98%)	131 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	7	32
41	DO	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
42	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
42	DP	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	48
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	48
44	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	3	19
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	45
46	CT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
46	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
47	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	11	43
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	11	43
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	2	14
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	6	28
49	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
49	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
50	CX	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
50	DX	75/76 (99%)	73 (97%)	2 (3%)	0	100	100
51	CY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	32
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	2	12
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	9	38

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
10	AJ	57	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AM	5	ALA
17	AQ	82	ALA
23	C2	5	ILE
27	C0	4	THR
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	57	VAL
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
17	BQ	82	ALA
29	CC	158	ALA
32	CE	82	GLY
32	CE	83	VAL
34	CG	119	ALA
34	CG	175	LYS
34	CG	176	LYS
35	CH	10	ALA
36	CJ	19	ASN
37	CK	81	ILE
38	CL	35	VAL
39	CM	29	LYS
39	CM	69	ARG
48	CV	7	ARG
48	CV	16	GLY
35	DH	11	ASN
36	DJ	19	ASN
48	DV	52	LEU
53	DI	91	ALA
7	AG	56	LYS
13	AM	7	ILE
13	AM	105	ASN
14	AN	38	ASP
22	C1	25	VAL
22	C1	27	SER
27	C0	14	ILE
2	BB	95	ARG
3	BC	61	ALA
5	BE	51	GLY
5	BE	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	BF	92	THR
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
14	BN	38	ASP
15	BO	88	ARG
19	BS	6	LYS
20	BT	5	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
34	CG	46	ALA
36	CJ	25	GLY
38	CL	108	ARG
47	CU	89	GLU
48	CV	17	LYS
48	CV	89	ASP
34	DG	46	ALA
36	DJ	25	GLY
38	DL	108	ARG
43	DQ	105	GLY
48	DV	89	ASP
2	AB	95	ARG
4	AD	197	GLU
5	AE	162	GLU
8	AH	66	PHE
11	AK	89	PRO
23	C2	51	GLU
24	C3	45	SER
26	C5	20	ASP
2	BB	127	ASP
5	BE	110	ALA
5	BE	157	ARG
8	BH	66	PHE
10	BJ	36	VAL
10	BJ	95	GLY
11	BK	89	PRO
13	BM	4	ILE
17	BQ	17	MET
17	BQ	70	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	BT	43	ASP
29	CC	197	ASN
32	CE	6	LYS
35	CH	11	ASN
39	CM	36	LYS
41	CO	118	ARG
41	CO	119	SER
32	DE	6	LYS
53	DI	70	GLU
53	DI	109	LYS
53	DI	130	PRO
2	AB	125	THR
2	AB	127	ASP
16	AP	45	GLU
22	C1	26	THR
2	BB	125	THR
4	BD	197	GLU
5	BE	24	THR
6	BF	99	ALA
16	BP	44	SER
35	CH	9	VAL
36	CJ	23	PRO
37	CK	25	LEU
43	CQ	105	GLY
45	CS	43	ASN
45	CS	48	LYS
36	DJ	23	PRO
38	DL	75	SER
45	DS	44	GLY
53	DI	88	HIS
14	AN	21	PHE
20	AT	43	ASP
8	BH	67	GLN
17	BQ	18	GLU
35	CH	8	LYS
52	CZ	62	GLY
37	DK	25	LEU
39	DM	36	LYS
47	DU	89	GLU
53	DI	108	VAL
3	BC	127	ARG
6	BF	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	BG	56	LYS
10	BJ	93	ALA
45	CS	53	PHE
5	BE	105	ILE
35	CH	118	PRO
36	CJ	32	GLY
35	DH	118	PRO
36	DJ	32	GLY
10	AJ	33	GLY
33	CF	62	GLY
33	DF	62	GLY
25	D4	18	GLY
33	DF	176	PRO
25	C4	18	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	169 (91%)	17 (9%)	9	33
2	BB	186/186 (100%)	169 (91%)	17 (9%)	9	33
3	AC	170/170 (100%)	154 (91%)	16 (9%)	8	32
3	BC	170/170 (100%)	154 (91%)	16 (9%)	8	32
4	AD	172/172 (100%)	163 (95%)	9 (5%)	21	55
4	BD	172/172 (100%)	162 (94%)	10 (6%)	18	51
5	AE	118/118 (100%)	100 (85%)	18 (15%)	3	14
5	BE	113/118 (96%)	90 (80%)	23 (20%)	1	7
6	AF	92/92 (100%)	82 (89%)	10 (11%)	6	26
6	BF	87/92 (95%)	72 (83%)	15 (17%)	2	11
7	AG	124/124 (100%)	108 (87%)	16 (13%)	4	19
7	BG	124/124 (100%)	106 (86%)	18 (14%)	3	15
8	AH	104/104 (100%)	88 (85%)	16 (15%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	104/104 (100%)	87 (84%)	17 (16%)	2	12
9	AI	105/105 (100%)	99 (94%)	6 (6%)	18	52
9	BI	105/105 (100%)	99 (94%)	6 (6%)	18	52
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	8	33
10	BJ	86/87 (99%)	73 (85%)	13 (15%)	3	14
11	AK	90/90 (100%)	89 (99%)	1 (1%)	65	83
11	BK	90/90 (100%)	84 (93%)	6 (7%)	15	46
12	AL	102/102 (100%)	93 (91%)	9 (9%)	9	35
12	BL	102/102 (100%)	89 (87%)	13 (13%)	4	20
13	AM	92/92 (100%)	84 (91%)	8 (9%)	9	35
13	BM	92/92 (100%)	85 (92%)	7 (8%)	12	41
14	AN	83/83 (100%)	82 (99%)	1 (1%)	63	82
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	73
15	AO	76/76 (100%)	70 (92%)	6 (8%)	11	39
15	BO	76/76 (100%)	70 (92%)	6 (8%)	11	39
16	AP	65/65 (100%)	63 (97%)	2 (3%)	35	68
16	BP	65/65 (100%)	60 (92%)	5 (8%)	12	40
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	21
17	BQ	74/74 (100%)	64 (86%)	10 (14%)	4	18
18	AR	48/48 (100%)	45 (94%)	3 (6%)	16	48
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	75
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	19
19	BS	70/70 (100%)	63 (90%)	7 (10%)	7	29
20	AT	65/65 (100%)	58 (89%)	7 (11%)	6	26
20	BT	65/65 (100%)	51 (78%)	14 (22%)	1	6
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7	28
21	BU	48/48 (100%)	44 (92%)	4 (8%)	10	37
22	C1	47/47 (100%)	46 (98%)	1 (2%)	47	75
22	D1	47/47 (100%)	47 (100%)	0	100	100
23	C2	45/46 (98%)	43 (96%)	2 (4%)	25	60
23	D2	45/46 (98%)	42 (93%)	3 (7%)	15	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	C3	38/38 (100%)	35 (92%)	3 (8%)	11	39
24	D3	38/38 (100%)	36 (95%)	2 (5%)	20	54
25	C4	51/51 (100%)	48 (94%)	3 (6%)	18	50
25	D4	51/51 (100%)	49 (96%)	2 (4%)	28	62
26	C5	34/34 (100%)	31 (91%)	3 (9%)	9	35
26	D5	34/34 (100%)	33 (97%)	1 (3%)	37	70
27	C0	48/48 (100%)	40 (83%)	8 (17%)	2	12
27	D0	49/48 (102%)	43 (88%)	6 (12%)	5	21
29	CC	216/216 (100%)	203 (94%)	13 (6%)	17	50
29	DC	216/216 (100%)	209 (97%)	7 (3%)	34	67
30	CD	163/163 (100%)	155 (95%)	8 (5%)	22	56
30	DD	163/163 (100%)	156 (96%)	7 (4%)	26	60
32	CE	165/165 (100%)	149 (90%)	16 (10%)	8	30
32	DE	165/165 (100%)	158 (96%)	7 (4%)	26	61
33	CF	148/148 (100%)	128 (86%)	20 (14%)	4	18
33	DF	148/148 (100%)	130 (88%)	18 (12%)	5	21
34	CG	137/137 (100%)	133 (97%)	4 (3%)	37	70
34	DG	137/137 (100%)	133 (97%)	4 (3%)	37	70
35	CH	114/114 (100%)	96 (84%)	18 (16%)	2	13
35	DH	114/114 (100%)	97 (85%)	17 (15%)	3	15
36	CJ	104/104 (100%)	98 (94%)	6 (6%)	18	51
36	DJ	104/104 (100%)	98 (94%)	6 (6%)	18	51
37	CK	116/116 (100%)	109 (94%)	7 (6%)	17	50
37	DK	116/116 (100%)	111 (96%)	5 (4%)	26	60
38	CL	103/104 (99%)	96 (93%)	7 (7%)	14	45
38	DL	104/104 (100%)	99 (95%)	5 (5%)	23	57
39	CM	103/103 (100%)	93 (90%)	10 (10%)	8	30
39	DM	103/103 (100%)	97 (94%)	6 (6%)	18	51
40	CN	108/108 (100%)	101 (94%)	7 (6%)	15	47
40	DN	109/108 (101%)	103 (94%)	6 (6%)	19	53
41	CO	100/102 (98%)	91 (91%)	9 (9%)	9	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DO	102/102 (100%)	95 (93%)	7 (7%)	14	45
42	CP	86/87 (99%)	76 (88%)	10 (12%)	5	23
42	DP	87/87 (100%)	81 (93%)	6 (7%)	14	45
43	CQ	99/99 (100%)	93 (94%)	6 (6%)	17	49
43	DQ	99/99 (100%)	96 (97%)	3 (3%)	36	69
44	CR	89/89 (100%)	84 (94%)	5 (6%)	19	52
44	DR	89/89 (100%)	86 (97%)	3 (3%)	32	66
45	CS	84/84 (100%)	77 (92%)	7 (8%)	10	37
45	DS	84/84 (100%)	81 (96%)	3 (4%)	31	65
46	CT	93/93 (100%)	87 (94%)	6 (6%)	15	47
46	DT	93/93 (100%)	90 (97%)	3 (3%)	34	67
47	CU	80/80 (100%)	71 (89%)	9 (11%)	5	24
47	DU	80/80 (100%)	77 (96%)	3 (4%)	29	63
48	CV	83/83 (100%)	77 (93%)	6 (7%)	13	43
48	DV	83/83 (100%)	78 (94%)	5 (6%)	17	50
49	CW	78/78 (100%)	74 (95%)	4 (5%)	21	55
49	DW	78/78 (100%)	75 (96%)	3 (4%)	29	63
50	CX	56/58 (97%)	53 (95%)	3 (5%)	20	53
50	DX	58/58 (100%)	55 (95%)	3 (5%)	21	55
51	CY	67/67 (100%)	63 (94%)	4 (6%)	17	50
51	DY	67/67 (100%)	64 (96%)	3 (4%)	24	59
52	CZ	54/54 (100%)	49 (91%)	5 (9%)	8	32
52	DZ	54/54 (100%)	51 (94%)	3 (6%)	19	52
53	DI	103/103 (100%)	93 (90%)	10 (10%)	8	30
All	All	9460/9477 (100%)	8707 (92%)	753 (8%)	11	38

All (753) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	117	LEU
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	183	VAL
2	AB	205	ASP
2	AB	207	ILE
2	AB	212	LEU
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	46	GLU
3	AC	55	ILE
3	AC	75	ILE
3	AC	107	ARG
3	AC	110	GLU
3	AC	121	THR
3	AC	128	VAL
3	AC	161	GLU
3	AC	162	ILE
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	207	ILE
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	28	ILE
4	AD	48	LEU
4	AD	143	VAL
4	AD	151	LYS
4	AD	181	THR
4	AD	194	ASP
5	AE	14	LYS
5	AE	43	ASN
5	AE	46	VAL
5	AE	74	VAL
5	AE	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AE	78	ASN
5	AE	81	LEU
5	AE	82	GLN
5	AE	94	VAL
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	134	ILE
5	AE	137	VAL
5	AE	148	ASN
5	AE	149	SER
5	AE	164	ILE
6	AF	36	ILE
6	AF	39	LEU
6	AF	62	MET
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	84	VAL
6	AF	89	VAL
6	AF	93	LYS
7	AG	18	PHE
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	40	GLU
7	AG	58	GLU
7	AG	59	LEU
7	AG	63	GLU
7	AG	70	ARG
7	AG	76	LYS
7	AG	83	SER
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	13	ARG
8	AH	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	AH	46	ILE
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	87	LYS
8	AH	90	ASP
8	AH	96	MET
8	AH	107	SER
8	AH	117	ARG
8	AH	129	VAL
9	AI	11	ARG
9	AI	36	GLU
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	96	SER
10	AJ	6	ILE
10	AJ	19	ASP
10	AJ	22	THR
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	22	HIS
12	AL	24	LEU
12	AL	33	VAL
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE
13	AM	27	LYS
13	AM	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AM	58	ASP
13	AM	63	PHE
13	AM	64	VAL
14	AN	80	SER
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	88	ARG
15	AO	89	ARG
16	AP	36	VAL
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	21	ILE
17	AQ	26	GLU
17	AQ	33	ILE
17	AQ	38	ILE
17	AQ	51	ASN
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	20	GLU
18	AR	33	ILE
18	AR	66	SER
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
19	AS	63	THR
20	AT	8	LYS
20	AT	23	SER
20	AT	24	ARG
20	AT	44	LYS
20	AT	48	GLN
20	AT	66	LEU
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AU	18	ARG
21	AU	20	LYS
21	AU	56	HIS
22	C1	10	ARG
23	C2	5	ILE
23	C2	47	VAL
24	C3	1	MET
24	C3	15	SER
24	C3	44	VAL
25	C4	13	ARG
25	C4	51	SER
25	C4	52	LYS
26	C5	16	ILE
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	5	ILE
27	C0	10	THR
27	C0	19	LYS
27	C0	36	VAL
27	C0	39	GLU
27	C0	45	ARG
27	C0	59	GLU
2	BB	44	GLU
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	117	LEU
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	183	VAL
2	BB	205	ASP
2	BB	207	ILE
2	BB	212	LEU
3	BC	3	GLN
3	BC	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BC	21	THR
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	75	ILE
3	BC	110	GLU
3	BC	121	THR
3	BC	152	GLU
3	BC	161	GLU
3	BC	162	ILE
3	BC	175	LEU
3	BC	185	ASN
3	BC	207	ILE
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	28	ILE
4	BD	48	LEU
4	BD	143	VAL
4	BD	173	VAL
4	BD	181	THR
4	BD	194	ASP
4	BD	206	LYS
5	BE	14	LYS
5	BE	19	ASN
5	BE	24	THR
5	BE	30	ILE
5	BE	43	ASN
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	105	ILE
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BE	137	VAL
5	BE	148	ASN
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	7	VAL
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	62	MET
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	74	LEU
6	BF	79	ARG
6	BF	84	VAL
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	40	GLU
7	BG	48	GLU
7	BG	50	LEU
7	BG	58	GLU
7	BG	59	LEU
7	BG	63	GLU
7	BG	70	ARG
7	BG	76	LYS
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	141	VAL
7	BG	142	HIS
8	BH	3	MET
8	BH	13	ARG
8	BH	46	ILE
8	BH	47	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BH	51	VAL
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	87	LYS
8	BH	90	ASP
8	BH	96	MET
8	BH	107	SER
8	BH	117	ARG
8	BH	129	VAL
9	BI	11	ARG
9	BI	36	GLU
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	96	SER
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	19	ASP
10	BJ	22	THR
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	77	VAL
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	65	VAL
11	BK	72	ASP
12	BL	4	VAL
12	BL	24	LEU
12	BL	33	VAL
12	BL	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	86	ARG
12	BL	88	LYS
12	BL	90	LEU
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	17	ILE
13	BM	22	ILE
13	BM	27	LYS
13	BM	41	GLU
13	BM	48	LEU
14	BN	26	GLU
14	BN	80	SER
15	BO	2	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	70	LEU
16	BP	19	VAL
16	BP	20	VAL
16	BP	36	VAL
16	BP	48	GLU
16	BP	76	LYS
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	33	ILE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	67	LEU
17	BQ	75	LEU
18	BR	33	ILE
19	BS	6	LYS
19	BS	7	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	BS	11	ILE
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG
19	BS	63	THR
20	BT	5	LYS
20	BT	12	ILE
20	BT	24	ARG
20	BT	27	MET
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
20	BT	86	LEU
21	BU	13	ASP
21	BU	16	LEU
21	BU	18	ARG
21	BU	56	HIS
23	D2	5	ILE
23	D2	8	LYS
23	D2	47	VAL
24	D3	1	MET
24	D3	15	SER
25	D4	47	LYS
25	D4	52	LYS
26	D5	16	ILE
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
27	D0	39	GLU
27	D0	58	GLU
29	CC	97	LYS
29	CC	110	LEU
29	CC	120	VAL
29	CC	156	ARG
29	CC	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	CC	168	ASP
29	CC	195	VAL
29	CC	202	LEU
29	CC	204	VAL
29	CC	205	LEU
29	CC	221	ARG
29	CC	236	GLU
29	CC	267	ILE
30	CD	2	ILE
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	73	VAL
30	CD	92	VAL
30	CD	95	SER
30	CD	138	LEU
29	DC	70	ASN
29	DC	97	LYS
29	DC	110	LEU
29	DC	120	VAL
29	DC	182	ARG
29	DC	202	LEU
29	DC	236	GLU
30	DD	2	ILE
30	DD	13	ARG
30	DD	18	ASP
30	DD	73	VAL
30	DD	92	VAL
30	DD	95	SER
30	DD	138	LEU
32	CE	7	ASP
32	CE	12	LEU
32	CE	25	GLU
32	CE	40	ARG
32	CE	44	ARG
32	CE	72	SER
32	CE	83	VAL
32	CE	93	SER
32	CE	107	SER
32	CE	120	VAL
32	CE	122	GLU
32	CE	127	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CE	149	ILE
32	CE	152	GLU
32	CE	163	ASN
32	CE	189	THR
33	CF	27	GLN
33	CF	31	VAL
33	CF	35	THR
33	CF	36	LEU
33	CF	49	LEU
33	CF	57	LEU
33	CF	72	LYS
33	CF	80	ARG
33	CF	89	VAL
33	CF	94	GLU
33	CF	117	LEU
33	CF	123	ASP
33	CF	134	GLU
33	CF	136	ILE
33	CF	141	ILE
33	CF	149	VAL
33	CF	150	ARG
33	CF	152	LEU
33	CF	167	ARG
33	CF	174	ASP
34	CG	11	VAL
34	CG	18	LYS
34	CG	72	LEU
34	CG	155	GLU
35	CH	1	MET
35	CH	7	ASP
35	CH	9	VAL
35	CH	15	LEU
35	CH	21	VAL
35	CH	51	ARG
35	CH	53	GLU
35	CH	54	LEU
35	CH	55	GLU
35	CH	58	LEU
35	CH	62	LEU
35	CH	75	LEU
35	CH	76	GLU
35	CH	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	CH	109	GLU
35	CH	112	LYS
35	CH	127	GLU
35	CH	145	ASN
36	CJ	13	VAL
36	CJ	28	LEU
36	CJ	53	LEU
36	CJ	55	ILE
36	CJ	101	ILE
36	CJ	113	LYS
37	CK	5	THR
37	CK	11	VAL
37	CK	30	THR
37	CK	39	LYS
37	CK	81	ILE
37	CK	124	VAL
37	CK	142	ILE
38	CL	35	VAL
38	CL	38	ILE
38	CL	58	LEU
38	CL	70	ARG
38	CL	76	VAL
38	CL	80	ASP
38	CL	113	MET
39	CM	21	ARG
39	CM	42	SER
39	CM	59	ARG
39	CM	92	LEU
39	CM	93	ASN
39	CM	94	THR
39	CM	100	ILE
39	CM	103	ILE
39	CM	116	VAL
39	CM	120	VAL
40	CN	55	ARG
40	CN	59	ARG
40	CN	75	GLU
40	CN	78	LEU
40	CN	115	GLU
40	CN	126	ILE
40	CN	132	THR
41	CO	2	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	CO	6	SER
41	CO	14	SER
41	CO	33	ILE
41	CO	69	ARG
41	CO	71	ARG
41	CO	76	VAL
41	CO	95	THR
41	CO	116	VAL
42	CP	18	LEU
42	CP	20	GLU
42	CP	31	THR
42	CP	38	GLN
42	CP	47	VAL
42	CP	48	LEU
42	CP	49	VAL
42	CP	78	VAL
42	CP	111	ARG
42	CP	115	LEU
43	CQ	2	SER
43	CQ	10	GLN
43	CQ	26	VAL
43	CQ	39	ARG
43	CQ	40	LEU
43	CQ	114	LEU
44	CR	5	LYS
44	CR	9	ILE
44	CR	16	LYS
44	CR	51	ARG
44	CR	52	GLN
45	CS	38	VAL
45	CS	45	GLU
45	CS	46	GLU
45	CS	48	LYS
45	CS	51	VAL
45	CS	58	VAL
45	CS	102	SER
46	CT	29	VAL
46	CT	69	LEU
46	CT	86	MET
46	CT	97	LEU
46	CT	108	SER
46	CT	109	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	CU	1	MET
47	CU	2	ILE
47	CU	18	GLU
47	CU	27	SER
47	CU	30	ILE
47	CU	49	LYS
47	CU	69	ARG
47	CU	74	ILE
47	CU	93	LEU
48	CV	28	VAL
48	CV	29	LEU
48	CV	61	LYS
48	CV	72	ILE
48	CV	81	ASP
48	CV	101	GLU
49	CW	1	MET
49	CW	7	GLU
49	CW	10	LYS
49	CW	61	LEU
50	CX	39	ARG
50	CX	40	GLN
50	CX	82	ILE
51	CY	25	THR
51	CY	44	LYS
51	CY	48	THR
51	CY	71	LEU
52	CZ	18	LEU
52	CZ	19	LEU
52	CZ	38	GLN
52	CZ	40	SER
52	CZ	58	ASN
32	DE	12	LEU
32	DE	25	GLU
32	DE	107	SER
32	DE	120	VAL
32	DE	127	GLU
32	DE	163	ASN
32	DE	189	THR
33	DF	10	ASP
33	DF	35	THR
33	DF	49	LEU
33	DF	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	DF	72	LYS
33	DF	89	VAL
33	DF	94	GLU
33	DF	115	ARG
33	DF	117	LEU
33	DF	134	GLU
33	DF	136	ILE
33	DF	141	ILE
33	DF	149	VAL
33	DF	150	ARG
33	DF	152	LEU
33	DF	158	THR
33	DF	167	ARG
33	DF	174	ASP
34	DG	11	VAL
34	DG	72	LEU
34	DG	155	GLU
34	DG	168	VAL
35	DH	1	MET
35	DH	7	ASP
35	DH	15	LEU
35	DH	21	VAL
35	DH	53	GLU
35	DH	54	LEU
35	DH	58	LEU
35	DH	60	GLU
35	DH	62	LEU
35	DH	75	LEU
35	DH	76	GLU
35	DH	89	LYS
35	DH	112	LYS
35	DH	116	ARG
35	DH	117	LEU
35	DH	127	GLU
35	DH	145	ASN
36	DJ	13	VAL
36	DJ	28	LEU
36	DJ	53	LEU
36	DJ	55	ILE
36	DJ	101	ILE
36	DJ	113	LYS
37	DK	9	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	DK	11	VAL
37	DK	84	ILE
37	DK	124	VAL
37	DK	142	ILE
38	DL	38	ILE
38	DL	58	LEU
38	DL	70	ARG
38	DL	80	ASP
38	DL	110	GLU
39	DM	59	ARG
39	DM	60	ARG
39	DM	92	LEU
39	DM	94	THR
39	DM	116	VAL
39	DM	120	VAL
40	DN	75	GLU
40	DN	78	LEU
40	DN	100	LYS
40	DN	115	GLU
40	DN	126	ILE
40	DN	132	THR
41	DO	2	ARG
41	DO	6	SER
41	DO	14	SER
41	DO	33	ILE
41	DO	69	ARG
41	DO	76	VAL
41	DO	116	VAL
42	DP	20	GLU
42	DP	31	THR
42	DP	49	VAL
42	DP	78	VAL
42	DP	111	ARG
42	DP	115	LEU
43	DQ	26	VAL
43	DQ	40	LEU
43	DQ	109	ARG
44	DR	5	LYS
44	DR	9	ILE
44	DR	51	ARG
45	DS	38	VAL
45	DS	45	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	DS	102	SER
46	DT	86	MET
46	DT	108	SER
46	DT	109	ASP
47	DU	1	MET
47	DU	25	GLU
47	DU	27	SER
48	DV	28	VAL
48	DV	29	LEU
48	DV	52	LEU
48	DV	61	LYS
48	DV	101	GLU
49	DW	7	GLU
49	DW	53	LYS
49	DW	61	LEU
50	DX	11	ARG
50	DX	39	ARG
50	DX	82	ILE
51	DY	25	THR
51	DY	44	LYS
51	DY	71	LEU
52	DZ	12	GLU
52	DZ	19	LEU
52	DZ	38	GLN
53	DI	16	SER
53	DI	31	ARG
53	DI	53	ARG
53	DI	60	LEU
53	DI	64	VAL
53	DI	82	ILE
53	DI	85	VAL
53	DI	107	GLU
53	DI	117	LEU
53	DI	123	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	42	ASN
2	AB	93	ASN
2	AB	120	GLN
2	AB	146	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	25	ASN
3	AC	69	HIS
3	AC	123	GLN
4	AD	152	GLN
5	AE	77	ASN
5	AE	89	HIS
6	AF	17	GLN
6	AF	55	HIS
6	AF	63	ASN
7	AG	86	GLN
7	AG	142	HIS
7	AG	148	ASN
8	AH	4	GLN
8	AH	38	ASN
8	AH	67	GLN
8	AH	76	GLN
9	AI	4	ASN
9	AI	110	GLN
9	AI	126	GLN
10	AJ	56	HIS
11	AK	40	ASN
11	AK	118	HIS
12	AL	77	HIS
13	AM	12	HIS
14	AN	4	GLN
14	AN	35	ASN
15	AO	62	GLN
16	AP	9	HIS
16	AP	40	ASN
17	AQ	51	ASN
18	AR	52	GLN
19	AS	57	HIS
20	AT	52	ASN
22	C1	6	ASN
22	C1	38	HIS
24	C3	13	ASN
25	C4	28	ASN
27	C0	9	GLN
2	BB	39	HIS
2	BB	42	ASN
2	BB	93	ASN
2	BB	146	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BC	25	ASN
3	BC	69	HIS
3	BC	123	GLN
4	BD	152	GLN
5	BE	77	ASN
5	BE	89	HIS
5	BE	122	ASN
6	BF	3	HIS
6	BF	17	GLN
6	BF	46	GLN
7	BG	148	ASN
8	BH	4	GLN
8	BH	67	GLN
9	BI	4	ASN
9	BI	5	GLN
9	BI	110	GLN
9	BI	126	GLN
10	BJ	56	HIS
11	BK	40	ASN
14	BN	4	GLN
14	BN	35	ASN
15	BO	40	GLN
15	BO	62	GLN
16	BP	40	ASN
17	BQ	45	HIS
17	BQ	51	ASN
18	BR	52	GLN
20	BT	48	GLN
20	BT	52	ASN
20	BT	61	GLN
24	D3	29	GLN
27	D0	20	HIS
29	CC	142	HIS
29	CC	153	GLN
29	CC	260	ASN
30	CD	49	GLN
30	CD	173	GLN
29	DC	142	HIS
30	DD	42	ASN
30	DD	49	GLN
32	CE	94	GLN
32	CE	115	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CE	136	GLN
32	CE	163	ASN
33	CF	23	ASN
33	CF	52	ASN
34	CG	38	ASN
34	CG	73	ASN
34	CG	104	ASN
34	CG	128	GLN
35	CH	2	GLN
35	CH	18	GLN
35	CH	20	ASN
35	CH	28	ASN
35	CH	43	ASN
36	CJ	43	ASN
37	CK	47	HIS
38	CL	5	GLN
38	CL	88	ASN
40	CN	13	HIS
40	CN	22	GLN
42	CP	116	GLN
43	CQ	41	GLN
45	CS	12	HIS
46	CT	9	HIS
48	CV	74	ASN
49	CW	24	ASN
52	CZ	45	GLN
32	DE	90	GLN
32	DE	94	GLN
33	DF	27	GLN
34	DG	104	ASN
34	DG	116	GLN
34	DG	128	GLN
35	DH	2	GLN
35	DH	18	GLN
35	DH	20	ASN
35	DH	43	ASN
36	DJ	43	ASN
37	DK	47	HIS
38	DL	88	ASN
38	DL	93	GLN
39	DM	35	HIS
41	DO	31	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	DO	107	ASN
42	DP	116	GLN
45	DS	87	GLN
46	DT	40	ASN
47	DU	70	HIS
48	DV	54	GLN
50	DX	12	ASN
52	DZ	45	GLN
53	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	259 (16%)	32 (2%)
1	BA	1532/1534 (99%)	260 (16%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	1 (0%)
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2896/2904 (99%)	485 (16%)	79 (2%)
54	DA	2884/2904 (99%)	406 (14%)	60 (2%)
All	All	9081/9116 (99%)	1432 (15%)	208 (2%)

All (1432) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	74	A
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	197	A
1	AA	200	G
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	298	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	305	G
1	AA	306	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	368	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	615	G
1	AA	632	U
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	682	G
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	873	A
1	AA	914	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	926	G
1	AA	927	G
1	AA	932	C
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1052	G
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
1	AA	1065	U
1	AA	1086	U
1	AA	1087	G
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1146	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1282	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1323	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1397	C
1	AA	1398	A
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1492	A
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	6	G
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	250	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	298	A
1	BA	305	G
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	368	U
1	BA	372	C
1	BA	373	A
1	BA	382	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	527	G7M
1	BA	528	C
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	561	U
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	579	A
1	BA	615	G
1	BA	632	U
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	682	G
1	BA	695	A
1	BA	702	A
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	812	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	818	G
1	BA	821	G
1	BA	828	U
1	BA	836	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	873	A
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	992	U
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1053	G
1	BA	1054	C
1	BA	1055	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1065	U
1	BA	1086	U
1	BA	1087	G
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1146	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1281	C
1	BA	1282	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1323	G
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1397	C
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	39	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	61	C
31	CA	63	A
31	CA	71	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	143	C
31	CA	165	A
31	CA	177	G
31	CA	178	G
31	CA	188	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	264	C
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	310	A
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	370	G
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	403	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	455	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	513	A
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	622	G
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	723	C
31	CA	730	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	764	A
31	CA	765	C
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	973	A
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1005	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1062	G
31	CA	1069	A
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1134	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1206	G
31	CA	1210	G
31	CA	1212	G
31	CA	1227	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1329	U
31	CA	1330	C
31	CA	1342	A
31	CA	1344	U
31	CA	1352	U
31	CA	1365	A
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1478	G
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1504	A
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1567	G
31	CA	1568	G
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1609	A
31	CA	1611	C
31	CA	1616	A
31	CA	1632	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1669	A
31	CA	1674	G
31	CA	1675	C
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1754	A
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U
31	CA	1816	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1834	U
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1971	U
31	CA	1972	G
31	CA	1975	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2006	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2046	G
31	CA	2049	G
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2120	G
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2280	G
31	CA	2282	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2324	U
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2334	U
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2484	G
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2579	C
31	CA	2582	G
31	CA	2585	U
31	CA	2586	U
31	CA	2592	G
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2623	G
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2716	C
31	CA	2718	G
31	CA	2720	U
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2765	A
31	CA	2769	U
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2825	G
31	CA	2833	U
31	CA	2835	A
31	CA	2836	U
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2880	C
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2903	U
28	DB	25	U
28	DB	35	C
28	DB	44	G
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C
28	DB	89	U
28	DB	90	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	DB	109	A
54	DA	10	A
54	DA	12	U
54	DA	14	A
54	DA	15	G
54	DA	34	U
54	DA	39	G
54	DA	42	A
54	DA	46	G
54	DA	58	G
54	DA	61	C
54	DA	63	A
54	DA	71	A
54	DA	74	A
54	DA	75	G
54	DA	84	A
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
54	DA	125	A
54	DA	138	U
54	DA	139	U
54	DA	140	C
54	DA	141	G
54	DA	142	A
54	DA	143	C
54	DA	165	A
54	DA	196	A
54	DA	197	A
54	DA	199	A
54	DA	200	U
54	DA	215	G
54	DA	216	A
54	DA	221	A
54	DA	222	A
54	DA	248	G
54	DA	264	C
54	DA	265	A
54	DA	266	G
54	DA	272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	276	U
54	DA	277	G
54	DA	278	A
54	DA	279	A
54	DA	285	G
54	DA	302	C
54	DA	311	A
54	DA	329	G
54	DA	330	A
54	DA	343	C
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	385	C
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A
54	DA	420	C
54	DA	424	G
54	DA	451	U
54	DA	480	A
54	DA	481	G
54	DA	491	G
54	DA	503	A
54	DA	504	A
54	DA	505	A
54	DA	508	A
54	DA	513	A
54	DA	528	A
54	DA	532	A
54	DA	533	G
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G
54	DA	550	C
54	DA	551	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	563	A
54	DA	573	U
54	DA	575	A
54	DA	586	A
54	DA	603	A
54	DA	613	A
54	DA	614	A
54	DA	615	U
54	DA	627	A
54	DA	637	A
54	DA	645	C
54	DA	647	G
54	DA	653	U
54	DA	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	C
54	DA	723	C
54	DA	730	A
54	DA	747	5MU
54	DA	764	A
54	DA	765	C
54	DA	775	G
54	DA	776	G
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	805	G
54	DA	812	C
54	DA	827	U
54	DA	828	U
54	DA	858	G
54	DA	859	G
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A
54	DA	931	U
54	DA	932	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	933	A
54	DA	946	C
54	DA	953	G
54	DA	961	C
54	DA	974	G
54	DA	983	A
54	DA	984	A
54	DA	985	C
54	DA	996	A
54	DA	1012	U
54	DA	1013	C
54	DA	1022	G
54	DA	1026	G
54	DA	1033	U
54	DA	1040	A
54	DA	1047	G
54	DA	1057	A
54	DA	1061	U
54	DA	1062	G
54	DA	1068	G
54	DA	1069	A
54	DA	1070	A
54	DA	1073	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1119	U
54	DA	1128	G
54	DA	1129	A
54	DA	1132	U
54	DA	1133	A
54	DA	1134	A
54	DA	1135	C
54	DA	1136	G
54	DA	1141	U
54	DA	1142	A
54	DA	1143	A
54	DA	1155	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1168	G
54	DA	1171	G
54	DA	1172	C
54	DA	1175	A
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1206	G
54	DA	1212	G
54	DA	1238	G
54	DA	1253	A
54	DA	1256	G
54	DA	1271	G
54	DA	1272	A
54	DA	1273	U
54	DA	1300	G
54	DA	1301	A
54	DA	1321	A
54	DA	1329	U
54	DA	1342	A
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1478	G
54	DA	1482	G
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1504	A
54	DA	1508	A
54	DA	1509	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1569	A
54	DA	1578	U
54	DA	1583	A
54	DA	1585	C
54	DA	1607	C
54	DA	1608	A
54	DA	1609	A
54	DA	1616	A
54	DA	1647	U
54	DA	1648	U
54	DA	1649	G
54	DA	1674	G
54	DA	1715	G
54	DA	1729	U
54	DA	1730	C
54	DA	1738	G
54	DA	1744	A
54	DA	1754	A
54	DA	1764	C
54	DA	1773	A
54	DA	1782	U
54	DA	1800	C
54	DA	1801	A
54	DA	1808	A
54	DA	1812	U
54	DA	1816	C
54	DA	1829	A
54	DA	1869	G
54	DA	1870	C
54	DA	1871	A
54	DA	1872	A
54	DA	1873	G
54	DA	1906	G
54	DA	1907	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1913	A
54	DA	1914	C
54	DA	1929	G
54	DA	1930	G
54	DA	1931	U
54	DA	1937	A
54	DA	1938	A
54	DA	1955	U
54	DA	1965	C
54	DA	1967	C
54	DA	1970	A
54	DA	1972	G
54	DA	1991	U
54	DA	1993	U
54	DA	1997	C
54	DA	2023	C
54	DA	2031	A
54	DA	2033	A
54	DA	2043	C
54	DA	2055	C
54	DA	2056	G
54	DA	2060	A
54	DA	2061	G
54	DA	2062	A
54	DA	2069	G7M
54	DA	2093	G
54	DA	2097	A
54	DA	2100	G
54	DA	2105	U
54	DA	2111	U
54	DA	2112	G
54	DA	2113	U
54	DA	2116	G
54	DA	2117	A
54	DA	2118	U
54	DA	2119	A
54	DA	2120	G
54	DA	2123	G
54	DA	2125	G
54	DA	2126	A
54	DA	2128	G
54	DA	2131	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2132	U
54	DA	2133	G
54	DA	2134	A
54	DA	2135	A
54	DA	2145	C
54	DA	2146	C
54	DA	2147	A
54	DA	2148	G
54	DA	2158	A
54	DA	2159	G
54	DA	2160	C
54	DA	2161	C
54	DA	2162	G
54	DA	2163	A
54	DA	2164	C
54	DA	2165	C
54	DA	2167	U
54	DA	2168	G
54	DA	2169	A
54	DA	2170	A
54	DA	2171	A
54	DA	2172	U
54	DA	2173	A
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2186	G
54	DA	2190	G
54	DA	2198	A
54	DA	2203	U
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G
54	DA	2268	A
54	DA	2278	A
54	DA	2280	G
54	DA	2283	C
54	DA	2286	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2311	A
54	DA	2312	U
54	DA	2322	A
54	DA	2324	U
54	DA	2325	G
54	DA	2327	A
54	DA	2331	G
54	DA	2335	A
54	DA	2345	G
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2406	A
54	DA	2407	A
54	DA	2423	U
54	DA	2424	C
54	DA	2425	A
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2465	C
54	DA	2474	U
54	DA	2476	A
54	DA	2484	G
54	DA	2491	U
54	DA	2502	G
54	DA	2505	G
54	DA	2518	A
54	DA	2529	G
54	DA	2535	G
54	DA	2547	A
54	DA	2556	C
54	DA	2566	A
54	DA	2567	G
54	DA	2573	C
54	DA	2585	U
54	DA	2586	U
54	DA	2603	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2609	U
54	DA	2613	U
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
54	DA	2716	C
54	DA	2726	A
54	DA	2744	G
54	DA	2748	A
54	DA	2765	A
54	DA	2778	A
54	DA	2791	G
54	DA	2798	U
54	DA	2799	A
54	DA	2818	U
54	DA	2820	A
54	DA	2821	A
54	DA	2825	G
54	DA	2833	U
54	DA	2835	A
54	DA	2836	U
54	DA	2867	G
54	DA	2880	C
54	DA	2883	A
54	DA	2903	U

All (208) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	30	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	305	G
1	AA	367	U
1	AA	413	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	422	C
1	AA	429	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1094	G
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1301	U
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	305	G
1	BA	367	U
1	BA	422	C
1	BA	429	U
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	844	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1301	U
1	BA	1362	A
1	BA	1363	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
28	CB	89	U
31	CA	33	C
31	CA	83	A
31	CA	138	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	371	A
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	503	A
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	775	G
31	CA	784	G
31	CA	827	U
31	CA	846	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1132	U
31	CA	1133	A
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1567	G
31	CA	1607	C
31	CA	1609	A
31	CA	1647	U
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1929	G
31	CA	1970	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2172	U
31	CA	2225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2282	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2581	G
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2820	A
31	CA	2849	U
31	CA	2873	A
54	DA	138	U
54	DA	141	G
54	DA	196	A
54	DA	199	A
54	DA	271	G
54	DA	278	A
54	DA	310	A
54	DA	370	G
54	DA	371	A
54	DA	403	U
54	DA	503	A
54	DA	620	G
54	DA	764	A
54	DA	784	G
54	DA	984	A
54	DA	1061	U
54	DA	1069	A
54	DA	1070	A
54	DA	1087	G
54	DA	1089	A
54	DA	1128	G
54	DA	1133	A
54	DA	1141	U
54	DA	1142	A
54	DA	1171	G
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1301	A
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A
54	DA	1535	A
54	DA	1607	C
54	DA	1609	A
54	DA	1647	U
54	DA	1870	C
54	DA	1871	A
54	DA	2062	A
54	DA	2097	A
54	DA	2119	A
54	DA	2127	G
54	DA	2146	C
54	DA	2157	G
54	DA	2158	A
54	DA	2164	C
54	DA	2172	U
54	DA	2286	G
54	DA	2311	A
54	DA	2324	U
54	DA	2406	A
54	DA	2423	U
54	DA	2585	U
54	DA	2779	U
54	DA	2798	U
54	DA	2820	A
54	DA	2873	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

77 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	BA	1207	1	23,26,27	0.30	0	33,38,41	0.42	0
54	3TD	DA	1915	54	19,22,23	0.46	0	23,32,35	0.85	1 (4%)
31	2MG	CA	1835	31	23,26,27	0.35	0	33,38,41	0.40	0
54	1MG	DA	745	54	23,26,27	0.90	2 (8%)	33,39,42	0.80	2 (6%)
1	G7M	AA	527	1	23,26,27	0.67	0	34,39,42	2.00	5 (14%)
54	PSU	DA	746	55,54	18,21,22	0.98	2 (11%)	21,30,33	0.34	0
31	6MZ	CA	1618	31	22,25,26	0.53	0	29,36,39	0.50	0
1	MA6	BA	1518	1	23,26,27	0.42	0	33,38,41	1.20	4 (12%)
54	OMC	DA	2498	55,54	19,22,23	0.54	0	25,31,34	0.54	0
54	6MZ	DA	1618	54	22,25,26	0.69	0	29,36,39	0.47	0
1	G7M	BA	527	1	23,26,27	0.62	0	34,39,42	1.86	5 (14%)
31	2MA	CA	2503	31	22,25,26	0.64	0	32,37,40	1.84	5 (15%)
40	4D4	DN	81[A]	-	9,11,12	2.22	2 (22%)	7,13,15	2.66	2 (28%)
54	2MG	DA	1835	54	23,26,27	0.30	0	33,38,41	0.39	0
31	3TD	CA	1915	31	19,22,23	0.48	0	23,32,35	0.83	1 (4%)
1	UR3	BA	1498	1	19,22,23	0.41	0	26,32,35	0.39	0
31	PSU	CA	746	31,55	18,21,22	0.58	1 (5%)	21,30,33	0.39	0
31	6MZ	CA	2030	31	22,25,26	0.53	0	29,36,39	0.57	0
54	PSU	DA	2604	54	18,21,22	0.94	1 (5%)	21,30,33	0.67	0
31	G7M	CA	2069	31	23,26,27	0.73	1 (4%)	34,39,42	1.99	5 (14%)
54	OMG	DA	2251	54	23,26,27	0.41	0	32,38,41	0.44	0
31	5MU	CA	1939	31	19,22,23	0.52	0	27,32,35	0.36	0
40	4D4	DN	81[B]	-	9,11,12	1.62	2 (22%)	7,13,15	2.83	2 (28%)
54	PSU	DA	1917	54	18,21,22	0.44	0	21,30,33	0.56	0
54	5MC	DA	1962	54	19,22,23	0.63	1 (5%)	26,32,35	0.47	0
31	2MG	CA	2445	31	23,26,27	0.39	0	33,38,41	0.48	0
31	OMU	CA	2552	31	19,22,23	0.30	0	25,31,34	0.29	0
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.42	0
54	2MA	DA	2503	55,54	22,25,26	0.66	0	32,37,40	1.55	5 (15%)
1	2MG	BA	1516	1	23,26,27	0.34	0	33,38,41	0.53	0
54	PSU	DA	2580	54	18,21,22	0.81	1 (5%)	21,30,33	0.76	1 (4%)
40	4D4	CN	81	40	9,11,12	2.18	2 (22%)	7,13,15	2.57	2 (28%)
1	MA6	AA	1519	1	23,26,27	0.56	0	33,38,41	1.20	4 (12%)
1	MA6	BA	1519	1	23,26,27	0.52	0	33,38,41	1.21	4 (12%)
1	2MG	AA	1207	1	23,26,27	0.23	0	33,38,41	0.34	0
1	UR3	AA	1498	1	19,22,23	0.69	0	26,32,35	0.46	0
31	1MG	CA	745	31	23,26,27	0.90	1 (4%)	33,39,42	0.81	2 (6%)
54	PSU	DA	1911	54	18,21,22	0.31	0	21,30,33	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	516	55,1	18,21,22	0.36	0	21,30,33	0.48	0
54	2MG	DA	2445	54	23,26,27	0.70	1 (4%)	33,38,41	0.49	0
1	2MG	BA	966	1	23,26,27	0.27	0	33,38,41	0.37	0
54	OMU	DA	2552	54	19,22,23	0.52	0	25,31,34	0.31	0
1	2MG	AA	966	1	23,26,27	0.32	0	33,38,41	0.48	0
1	4OC	BA	1402	1	20,23,24	0.38	0	25,32,35	0.44	0
30	MEQ	DD	150[A]	30	8,9,10	0.47	0	5,10,12	0.48	0
31	OMG	CA	2251	31	23,26,27	0.38	0	32,38,41	0.44	0
54	5MU	DA	1939	54	19,22,23	0.63	0	27,32,35	0.48	0
31	PSU	CA	2457	31	18,21,22	0.62	0	21,30,33	0.44	0
31	PSU	CA	2605	31	18,21,22	0.40	0	21,30,33	0.61	0
31	PSU	CA	955	31	18,21,22	0.34	0	21,30,33	0.55	0
1	5MC	BA	1407	1	19,22,23	0.48	0	26,32,35	0.47	0
1	5MC	AA	967	1	19,22,23	0.28	0	26,32,35	0.37	0
30	MEQ	DD	150[B]	30	8,9,10	1.35	1 (12%)	5,10,12	0.84	0
12	D2T	BL	89	12	8,9,10	1.09	1 (12%)	6,11,13	1.23	0
1	5MC	BA	967	1	19,22,23	0.26	0	26,32,35	0.37	0
12	D2T	AL	89	12	8,9,10	1.43	2 (25%)	6,11,13	1.29	0
54	PSU	DA	2457	54	18,21,22	0.52	0	21,30,33	0.48	0
31	5MU	CA	747	31	19,22,23	0.31	0	27,32,35	0.31	0
1	2MG	AA	1516	1	23,26,27	0.36	0	33,38,41	0.59	0
31	PSU	CA	2604	31	18,21,22	1.81	2 (11%)	21,30,33	1.48	3 (14%)
1	PSU	BA	516	1	18,21,22	0.42	0	21,30,33	0.46	0
31	5MC	CA	1962	31	19,22,23	0.28	0	26,32,35	0.42	0
31	PSU	CA	1917	31	18,21,22	0.32	0	21,30,33	0.50	0
54	PSU	DA	2504	54	18,21,22	0.47	0	21,30,33	0.41	0
54	PSU	DA	955	54	18,21,22	0.54	0	21,30,33	0.66	0
31	PSU	CA	2504	31	18,21,22	0.38	0	21,30,33	0.43	0
31	PSU	CA	2580	31	18,21,22	0.47	0	21,30,33	0.63	0
1	MA6	AA	1518	1	23,26,27	0.47	0	33,38,41	1.17	4 (12%)
54	G7M	DA	2069	54	23,26,27	0.74	1 (4%)	34,39,42	1.62	4 (11%)
54	H2U	DA	2449	54	18,21,22	0.58	0	19,30,33	0.53	0
54	PSU	DA	2605	54	18,21,22	0.62	0	21,30,33	0.67	0
54	6MZ	DA	2030	54	22,25,26	0.73	1 (4%)	29,36,39	0.62	0
54	5MU	DA	747	54	19,22,23	0.39	0	27,32,35	0.39	0
31	OMC	CA	2498	31,55	19,22,23	0.41	0	25,31,34	0.50	0
30	MEQ	CD	150	30	7,8,10	0.44	0	4,9,12	0.41	0
31	PSU	CA	1911	31	18,21,22	0.26	0	21,30,33	0.39	0
1	5MC	AA	1407	1	19,22,23	0.52	0	26,32,35	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	2/9/27/28	0/3/3/3
54	1MG	DA	745	54	-	0/7/25/26	0/3/3/3
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
54	PSU	DA	746	55,54	-	2/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
54	OMC	DA	2498	55,54	-	0/9/27/28	0/2/2/2
54	6MZ	DA	1618	54	-	0/9/27/28	0/3/3/3
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
31	2MA	CA	2503	31	-	0/7/25/26	0/3/3/3
40	4D4	DN	81[A]	-	-	2/11/12/14	-
54	2MG	DA	1835	54	-	2/9/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	746	31,55	-	2/7/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	1/9/27/28	0/3/3/3
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	0/7/25/26	0/3/3/3
54	OMG	DA	2251	54	-	0/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
40	4D4	DN	81[B]	-	-	6/11/12/14	-
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	5MC	DA	1962	54	-	2/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/9/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
54	2MA	DA	2503	55,54	-	0/7/25/26	0/3/3/3
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
40	4D4	CN	81	40	-	2/11/12/14	-
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	55,1	-	0/7/25/26	0/2/2/2
54	2MG	DA	2445	54	-	2/9/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
54	OMU	DA	2552	54	-	0/9/27/28	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
30	MEQ	DD	150[A]	30	-	4/8/9/11	-
31	OMG	CA	2251	31	-	0/9/27/28	0/3/3/3
54	5MU	DA	1939	54	-	0/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[B]	30	-	3/8/9/11	-
12	D2T	BL	89	12	-	4/7/12/14	-
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	1/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
31	PSU	CA	2604	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
54	G7M	DA	2069	54	-	0/7/25/26	0/3/3/3
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
54	6MZ	DA	2030	54	-	1/9/27/28	0/3/3/3
54	5MU	DA	747	54	-	2/7/25/26	0/2/2/2
31	OMC	CA	2498	31,55	-	0/9/27/28	0/2/2/2
30	MEQ	CD	150	30	-	3/6/7/11	-
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2604	PSU	C2-N1	6.14	1.44	1.36
40	CN	81	4D4	CZ-NE	5.94	1.44	1.33
40	DN	81[A]	4D4	CZ-NE	5.93	1.44	1.33
40	DN	81[B]	4D4	CZ-NE	4.08	1.41	1.33
31	CA	745	1MG	C2-N1	3.78	1.44	1.37
30	DD	150[B]	MEQ	CB-CA	3.62	1.59	1.53
54	DA	746	PSU	O4'-C1'	-3.10	1.39	1.43
31	CA	2604	PSU	C6-C5	2.82	1.38	1.35
12	AL	89	D2T	CB-SB	2.81	1.85	1.82
40	DN	81[A]	4D4	CZ-NH1	2.70	1.44	1.34
54	DA	745	1MG	C2-N1	2.59	1.42	1.37
54	DA	745	1MG	O3'-C3'	-2.57	1.36	1.43
12	BL	89	D2T	CB-CG	2.50	1.56	1.52
40	CN	81	4D4	CZ-NH1	2.39	1.43	1.34
54	DA	2604	PSU	O3'-C3'	-2.38	1.37	1.43
54	DA	746	PSU	C2'-C1'	-2.35	1.50	1.53
40	DN	81[B]	4D4	CZ-NH1	2.30	1.42	1.34
54	DA	1962	5MC	O5'-C5'	-2.24	1.37	1.44
54	DA	2069	G7M	C1'-N9	-2.23	1.41	1.47
54	DA	2580	PSU	O4'-C1'	-2.20	1.40	1.43
31	CA	2069	G7M	C1'-N9	-2.13	1.41	1.47
54	DA	2445	2MG	O3'-C3'	-2.13	1.37	1.43
12	AL	89	D2T	CB-CG	2.05	1.55	1.52
31	CA	746	PSU	O4'-C1'	-2.01	1.41	1.43
54	DA	2030	6MZ	O4'-C1'	-2.01	1.37	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	N6-C6-N1	8.03	127.86	117.03
31	CA	2069	G7M	C6-C5-N7	-7.41	122.88	132.17
1	AA	527	G7M	C6-C5-N7	-6.56	123.95	132.17
1	BA	527	G7M	C6-C5-N7	-6.39	124.16	132.17
54	DA	2503	2MA	N6-C6-N1	6.14	125.31	117.03
54	DA	2069	G7M	C6-C5-N7	-6.10	124.53	132.17
40	DN	81[B]	4D4	NE-CZ-NH2	6.09	131.13	120.67
40	DN	81[A]	4D4	NE-CZ-NH2	5.90	130.81	120.67
40	CN	81	4D4	NE-CZ-NH2	5.75	130.54	120.67
1	AA	527	G7M	C5-C4-N3	-5.67	117.43	128.15
31	CA	2069	G7M	C6-C5-C4	-5.43	109.61	119.01
31	CA	2069	G7M	C5-C4-N3	-4.60	119.46	128.15
1	BA	527	G7M	C6-C5-C4	-4.52	111.19	119.01
1	AA	527	G7M	O4'-C1'-N9	4.42	118.38	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	527	G7M	O4'-C1'-N9	4.40	118.33	108.36
31	CA	2604	PSU	C6-C5-C4	4.24	121.04	118.17
1	BA	527	G7M	C5-C4-N3	-4.22	120.17	128.15
54	DA	2069	G7M	C5-C4-N3	-4.21	120.19	128.15
40	DN	81[B]	4D4	NH1-CZ-NE	-4.07	110.01	119.27
31	CA	2503	2MA	C2-N1-C6	4.05	124.33	118.10
1	AA	1519	MA6	N1-C6-N6	-3.99	111.99	116.86
1	BA	1518	MA6	C4-C5-C6	-3.80	111.98	115.91
54	DA	2503	2MA	C2-N1-C6	3.78	123.92	118.10
1	BA	1519	MA6	C4-C5-C6	-3.74	112.04	115.91
1	BA	1519	MA6	N1-C6-N6	-3.67	112.39	116.86
1	AA	1518	MA6	C4-C5-C6	-3.65	112.14	115.91
1	AA	527	G7M	C4-C5-N7	-3.58	101.81	107.67
1	AA	527	G7M	C6-C5-C4	-3.54	112.89	119.01
1	AA	1519	MA6	C4-C5-C6	-3.51	112.28	115.91
31	CA	2604	PSU	C6-N1-C2	-3.47	119.47	122.69
54	DA	1915	3TD	C1'-C5-C4	3.43	122.81	117.61
31	CA	1915	3TD	C1'-C5-C4	3.34	122.68	117.61
40	DN	81[A]	4D4	NH1-CZ-NE	-3.34	111.68	119.27
1	AA	1518	MA6	N1-C6-N6	-3.32	112.81	116.86
1	BA	1518	MA6	N1-C6-N6	-3.32	112.81	116.86
54	DA	2069	G7M	C4-C5-N7	-3.29	102.29	107.67
1	BA	527	G7M	C4-C5-N7	-3.28	102.30	107.67
54	DA	2069	G7M	O4'-C1'-N9	3.24	115.70	108.36
31	CA	2069	G7M	O4'-C1'-N9	3.23	115.69	108.36
31	CA	745	1MG	N2-C2-N1	-3.14	116.26	118.79
31	CA	2069	G7M	C4-C5-N7	-3.06	102.67	107.67
40	CN	81	4D4	NH1-CZ-NE	-2.90	112.67	119.27
54	DA	745	1MG	N2-C2-N1	-2.90	116.46	118.79
1	BA	1518	MA6	C5-C6-N1	2.66	124.06	118.55
1	AA	1518	MA6	C5-C6-N1	2.61	123.97	118.55
1	BA	1519	MA6	C5-C6-N1	2.61	123.97	118.55
31	CA	2503	2MA	C5-C6-N1	-2.57	114.91	118.90
54	DA	745	1MG	C6-C5-C4	-2.56	117.08	119.97
1	AA	1519	MA6	C5-C6-N1	2.54	123.83	118.55
1	BA	1518	MA6	C6-C5-N7	2.52	137.46	133.43
31	CA	2604	PSU	O2-C2-N1	2.45	125.31	122.79
31	CA	2503	2MA	C5-C6-N6	-2.45	117.22	123.29
31	CA	745	1MG	C6-C5-C4	-2.37	117.29	119.97
54	DA	2503	2MA	CM2-C2-N3	2.34	120.62	117.13
1	AA	1518	MA6	C6-C5-N7	2.33	137.15	133.43
1	BA	1519	MA6	C6-C5-N7	2.33	137.15	133.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	2503	2MA	C5-C6-N1	-2.32	115.29	118.90
54	DA	2503	2MA	N3-C2-N1	-2.22	121.85	125.77
31	CA	2503	2MA	N3-C2-N1	-2.19	121.90	125.77
1	AA	1519	MA6	C6-C5-N7	2.14	136.84	133.43
54	DA	2580	PSU	O4'-C1'-C2'	2.10	108.05	105.15

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	O4'-C4'-C5'-O5'
40	DN	81[B]	4D4	C-CA-CB-OB
40	DN	81[B]	4D4	C-CA-CB-CG
40	DN	81[B]	4D4	N-CA-CB-CG
40	DN	81[B]	4D4	CA-CB-CG-CD
30	CD	150	MEQ	C-CA-CB-CG
30	DD	150[A]	MEQ	C-CA-CB-CG
30	DD	150[B]	MEQ	N-CA-CB-CG
30	DD	150[B]	MEQ	C-CA-CB-CG
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
30	CD	150	MEQ	CA-CB-CG-CD
40	DN	81[B]	4D4	OB-CB-CG-CD
30	DD	150[A]	MEQ	OE1-CD-CG-CB
30	DD	150[B]	MEQ	CA-CB-CG-CD
30	DD	150[A]	MEQ	NE2-CD-CG-CB
54	DA	747	5MU	C3'-C4'-C5'-O5'
31	CA	747	5MU	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
54	DA	2445	2MG	C3'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CG-CB-SB-CB1
30	CD	150	MEQ	N-CA-CB-CG
30	DD	150[A]	MEQ	N-CA-CB-CG
31	CA	1835	2MG	C3'-C4'-C5'-O5'
40	DN	81[A]	4D4	CG-CD-NE-CZ
54	DA	1835	2MG	C3'-C4'-C5'-O5'
54	DA	2030	6MZ	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	BL	89	D2T	SB-CB-CG-OD2
54	DA	2449	H2U	C4'-C5'-O5'-P
31	CA	1835	2MG	O4'-C4'-C5'-O5'
31	CA	746	PSU	O4'-C1'-C5-C6
54	DA	746	PSU	O4'-C1'-C5-C6
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	746	PSU	C2'-C1'-C5-C6
40	DN	81[B]	4D4	N-CA-CB-OB
54	DA	746	PSU	C2'-C1'-C5-C6
54	DA	2445	2MG	O4'-C4'-C5'-O5'
54	DA	1962	5MC	O4'-C1'-N1-C6
54	DA	1962	5MC	C2'-C1'-N1-C6
40	CN	81	4D4	O-C-CA-CB
40	DN	81[A]	4D4	O-C-CA-CB
1	BA	1402	4OC	O4'-C4'-C5'-O5'
54	DA	1835	2MG	O4'-C4'-C5'-O5'
31	CA	1618	6MZ	C4'-C5'-O5'-P
40	CN	81	4D4	CG-CD-NE-CZ
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
54	DA	747	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	1518	MA6	2	0
54	DA	2498	OMC	1	0
31	CA	2503	2MA	1	0
31	CA	1915	3TD	1	0
31	CA	2030	6MZ	3	0
54	DA	2251	OMG	1	0
31	CA	1939	5MU	1	0
1	AA	1402	4OC	1	0
1	AA	1519	MA6	2	0
1	BA	1519	MA6	2	0
1	BA	1402	4OC	1	0
30	DD	150[A]	MEQ	2	0
1	AA	967	5MC	1	0
30	DD	150[B]	MEQ	2	0
12	AL	89	D2T	1	0
31	CA	747	5MU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	CA	2580	PSU	1	0
1	AA	1518	MA6	2	0
54	DA	2030	6MZ	1	0
54	DA	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 559 ligands modelled in this entry, 475 are monoatomic - leaving 84 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.17	0
61	PEG	DA	3218	-	6,6,6	0.25	0	5,5,5	0.09	0
56	PG4	DA	3216	-	12,12,12	0.18	0	11,11,11	0.23	0
57	MPD	DT	201	-	7,7,7	0.48	0	9,10,10	0.25	0
62	EDO	DB	201	-	3,3,3	0.62	0	2,2,2	0.20	0
63	PGE	DA	3203	-	9,9,9	0.31	0	8,8,8	0.27	0
58	PUT	DM	201	-	5,5,5	0.14	0	4,4,4	0.06	0
57	MPD	AA	1676	-	7,7,7	0.71	0	9,10,10	0.76	0
58	PUT	DA	3223	-	5,5,5	0.24	0	4,4,4	0.16	0
59	TAC	BA	1644	55	34,35,35	0.58	0	43,58,58	0.92	2 (4%)
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.34	0
57	MPD	DN	201	-	7,7,7	0.88	0	9,10,10	0.54	0
63	PGE	DA	3225	-	9,9,9	0.17	0	8,8,8	0.15	0
56	PG4	DR	202	-	12,12,12	0.29	0	11,11,11	0.38	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.36	0
58	PUT	DA	3205	-	5,5,5	0.20	0	4,4,4	0.21	0
62	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.29	0
58	PUT	DA	3184	-	5,5,5	0.44	0	4,4,4	0.29	0
58	PUT	AA	1674	-	5,5,5	0.16	0	4,4,4	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TAC	AA	1680	55	34,35,35	0.53	0	43,58,58	1.12	2 (4%)
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.14	0
58	PUT	DA	3195	-	5,5,5	0.39	0	4,4,4	0.65	0
57	MPD	DT	202	-	7,7,7	0.73	0	9,10,10	0.38	0
58	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.12	0
66	ACY	DA	3196	-	3,3,3	2.46	1 (33%)	3,3,3	2.20	2 (66%)
58	PUT	AA	1675	-	5,5,5	0.18	0	4,4,4	0.10	0
58	PUT	DA	3221	-	5,5,5	0.21	0	4,4,4	0.17	0
63	PGE	DA	3186	-	9,9,9	0.38	0	8,8,8	0.44	0
56	PG4	DQ	202	-	12,12,12	0.21	0	11,11,11	0.16	0
56	PG4	DA	3193	-	12,12,12	0.41	0	11,11,11	0.34	0
61	PEG	DA	3227	-	6,6,6	0.27	0	5,5,5	0.17	0
58	PUT	DA	3222	-	5,5,5	0.53	0	4,4,4	0.74	0
64	SPD	DA	3183	-	9,9,9	0.10	0	8,8,8	0.14	0
62	EDO	DA	3197	-	3,3,3	0.70	0	2,2,2	0.13	0
58	PUT	AA	1673	-	5,5,5	0.13	0	4,4,4	0.09	0
57	MPD	DA	3190	-	7,7,7	0.33	0	9,10,10	0.44	0
62	EDO	D1	101	-	3,3,3	0.67	0	2,2,2	0.08	0
57	MPD	DA	3210	-	7,7,7	0.72	0	9,10,10	0.32	0
58	PUT	DA	3213	-	5,5,5	0.20	0	4,4,4	0.25	0
62	EDO	DA	3215	-	3,3,3	0.71	0	2,2,2	0.17	0
61	PEG	DQ	201	-	6,6,6	0.18	0	5,5,5	0.17	0
62	EDO	DA	3198	-	3,3,3	0.54	0	2,2,2	0.41	0
61	PEG	DA	3199	-	6,6,6	0.23	0	5,5,5	0.16	0
62	EDO	DB	212	-	3,3,3	0.71	0	2,2,2	0.13	0
68	TRS	DA	3220	-	7,7,7	0.34	0	9,9,9	0.37	0
64	SPD	DA	3224	-	9,9,9	0.24	0	8,8,8	0.48	0
57	MPD	DA	3207	-	7,7,7	0.75	0	9,10,10	0.51	0
58	PUT	DA	3189	-	5,5,5	0.25	0	4,4,4	0.39	0
62	EDO	DA	3003	-	3,3,3	0.56	0	2,2,2	0.26	0
61	PEG	DA	3200	-	6,6,6	0.39	0	5,5,5	0.22	0
61	PEG	DA	3226	-	6,6,6	0.45	0	5,5,5	0.19	0
63	PGE	DA	3214	-	9,9,9	0.30	0	8,8,8	0.41	0
62	EDO	DA	3002	-	3,3,3	0.56	0	2,2,2	0.39	0
63	PGE	DA	3001	-	9,9,9	0.32	0	8,8,8	0.32	0
64	SPD	DA	3187	-	9,9,9	0.19	0	8,8,8	0.33	0
57	MPD	DE	301	-	7,7,7	0.73	0	9,10,10	0.56	0
57	MPD	DA	3204	-	7,7,7	0.76	0	9,10,10	0.67	0
61	PEG	D3	101	-	6,6,6	0.29	0	5,5,5	0.29	0
61	PEG	D1	103	-	6,6,6	0.38	0	5,5,5	0.19	0
58	PUT	DA	3212	-	5,5,5	0.25	0	4,4,4	0.07	0
62	EDO	DB	211	-	3,3,3	0.60	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	SPD	DA	3206	-	9,9,9	0.25	0	8,8,8	0.26	0
65	1PE	DA	3202	-	15,15,15	0.36	0	14,14,14	0.36	0
57	MPD	AA	1671	-	7,7,7	0.60	0	9,10,10	0.56	0
59	TAC	BA	1643	55	34,35,35	0.47	0	43,58,58	0.99	3 (6%)
66	ACY	DA	3201	-	3,3,3	0.66	0	3,3,3	1.03	0
61	PEG	AL	201	-	6,6,6	0.32	0	5,5,5	0.17	0
62	EDO	DA	3209	-	3,3,3	0.59	0	2,2,2	0.31	0
57	MPD	DA	3192	-	7,7,7	0.38	0	9,10,10	0.70	0
57	MPD	DE	302	-	7,7,7	0.85	0	9,10,10	0.59	0
63	PGE	DS	201	-	9,9,9	0.40	0	8,8,8	0.31	0
63	PGE	DU	101	-	9,9,9	0.21	0	8,8,8	0.13	0
62	EDO	DA	3194	-	3,3,3	0.88	0	2,2,2	0.12	0
59	TAC	AA	1681	55	34,35,35	0.56	0	43,58,58	0.94	3 (6%)
63	PGE	DA	3217	-	9,9,9	0.19	0	8,8,8	0.25	0
56	PG4	AA	1670	-	12,12,12	0.33	0	11,11,11	0.41	0
66	ACY	DA	3191	-	3,3,3	0.96	0	3,3,3	0.99	0
67	GUN	DA	3211	-	12,12,12	0.37	0	15,17,17	0.44	0
57	MPD	DS	203	-	7,7,7	0.23	0	9,10,10	0.39	0
58	PUT	AA	1672	-	5,5,5	0.25	0	4,4,4	0.30	0
57	MPD	DK	201	-	7,7,7	0.48	0	9,10,10	0.25	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.16	0
63	PGE	D1	102	-	9,9,9	0.24	0	8,8,8	0.22	0
58	PUT	DA	3188	-	5,5,5	0.24	0	4,4,4	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PG4	BA	1642	-	-	0/10/10/10	-
61	PEG	DA	3218	-	-	2/4/4/4	-
56	PG4	DA	3216	-	-	4/10/10/10	-
57	MPD	DT	201	-	-	3/5/5/5	-
62	EDO	DB	201	-	-	0/1/1/1	-
63	PGE	DA	3203	-	-	4/7/7/7	-
58	PUT	DM	201	-	-	0/3/3/3	-
57	MPD	AA	1676	-	-	2/5/5/5	-
58	PUT	DA	3223	-	-	1/3/3/3	-
59	TAC	BA	1644	55	-	6/8/74/74	0/4/4/4
56	PG4	DS	202	-	-	4/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DN	201	-	-	3/5/5/5	-
63	PGE	DA	3225	-	-	5/7/7/7	-
56	PG4	DR	202	-	-	5/10/10/10	-
65	1PE	DA	3185	-	-	5/13/13/13	-
58	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3208	-	-	1/1/1/1	-
58	PUT	DA	3184	-	-	0/3/3/3	-
58	PUT	AA	1674	-	-	0/3/3/3	-
59	TAC	AA	1680	55	-	1/8/74/74	0/4/4/4
61	PEG	DL	201	-	-	1/4/4/4	-
58	PUT	DA	3195	-	-	0/3/3/3	-
57	MPD	DT	202	-	-	3/5/5/5	-
58	PUT	DA	3219	-	-	0/3/3/3	-
58	PUT	AA	1675	-	-	1/3/3/3	-
58	PUT	DA	3221	-	-	0/3/3/3	-
63	PGE	DA	3186	-	-	2/7/7/7	-
56	PG4	DQ	202	-	-	3/10/10/10	-
56	PG4	DA	3193	-	-	7/10/10/10	-
61	PEG	DA	3227	-	-	0/4/4/4	-
58	PUT	DA	3222	-	-	0/3/3/3	-
64	SPD	DA	3183	-	-	1/7/7/7	-
62	EDO	DA	3197	-	-	1/1/1/1	-
58	PUT	AA	1673	-	-	0/3/3/3	-
57	MPD	DA	3190	-	-	1/5/5/5	-
62	EDO	D1	101	-	-	0/1/1/1	-
57	MPD	DA	3210	-	-	0/5/5/5	-
58	PUT	DA	3213	-	-	0/3/3/3	-
62	EDO	DA	3215	-	-	0/1/1/1	-
61	PEG	DQ	201	-	-	1/4/4/4	-
62	EDO	DA	3198	-	-	0/1/1/1	-
61	PEG	DA	3199	-	-	1/4/4/4	-
62	EDO	DB	212	-	-	1/1/1/1	-
68	TRS	DA	3220	-	-	0/9/9/9	-
64	SPD	DA	3224	-	-	3/7/7/7	-
57	MPD	DA	3207	-	-	3/5/5/5	-
58	PUT	DA	3189	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-
61	PEG	DA	3200	-	-	2/4/4/4	-
61	PEG	DA	3226	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DA	3214	-	-	3/7/7/7	-
62	EDO	DA	3002	-	-	1/1/1/1	-
63	PGE	DA	3001	-	-	4/7/7/7	-
64	SPD	DA	3187	-	-	2/7/7/7	-
57	MPD	DE	301	-	-	3/5/5/5	-
57	MPD	DA	3204	-	-	4/5/5/5	-
61	PEG	D3	101	-	-	2/4/4/4	-
61	PEG	D1	103	-	-	1/4/4/4	-
58	PUT	DA	3212	-	-	1/3/3/3	-
62	EDO	DB	211	-	-	0/1/1/1	-
64	SPD	DA	3206	-	-	2/7/7/7	-
65	1PE	DA	3202	-	-	7/13/13/13	-
57	MPD	AA	1671	-	-	1/5/5/5	-
59	TAC	BA	1643	55	-	8/8/74/74	0/4/4/4
61	PEG	AL	201	-	-	2/4/4/4	-
62	EDO	DA	3209	-	-	0/1/1/1	-
57	MPD	DA	3192	-	-	2/5/5/5	-
57	MPD	DE	302	-	-	2/5/5/5	-
63	PGE	DS	201	-	-	2/7/7/7	-
63	PGE	DU	101	-	-	3/7/7/7	-
62	EDO	DA	3194	-	-	0/1/1/1	-
59	TAC	AA	1681	55	-	6/8/74/74	0/4/4/4
63	PGE	DA	3217	-	-	2/7/7/7	-
56	PG4	AA	1670	-	-	4/10/10/10	-
67	GUN	DA	3211	-	-	-	0/2/2/2
57	MPD	DS	203	-	-	0/5/5/5	-
58	PUT	AA	1672	-	-	0/3/3/3	-
57	MPD	DK	201	-	-	3/5/5/5	-
61	PEG	DP	201	-	-	3/4/4/4	-
63	PGE	D1	102	-	-	5/7/7/7	-
58	PUT	DA	3188	-	-	0/3/3/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.09	1.40	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AA	1680	TAC	C5-C41-C4	-5.44	105.87	113.73
59	BA	1643	TAC	C5-C41-C4	-3.96	108.01	113.73
59	AA	1681	TAC	C5-C41-C4	-3.29	108.98	113.73
59	BA	1644	TAC	O3-C3-C2	-3.13	117.69	122.93
59	BA	1644	TAC	C5-C41-C4	-2.96	109.46	113.73
66	DA	3196	ACY	OXT-C-CH3	2.80	126.81	115.05
59	AA	1681	TAC	O3-C3-C2	-2.76	118.32	122.93
66	DA	3196	ACY	O-C-CH3	-2.57	112.00	122.53
59	BA	1643	TAC	O3-C3-C2	-2.25	119.16	122.93
59	AA	1681	TAC	C42-N4-C4	2.22	119.17	114.10
59	AA	1680	TAC	O3-C3-C2	-2.16	119.32	122.93
59	BA	1643	TAC	C11-C1B-C12	2.10	120.46	118.80

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1676	MPD	C2-C3-C4-C5
59	AA	1681	TAC	C1-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-N21
59	AA	1681	TAC	C41-C4-N4-C42
59	BA	1643	TAC	C1-C2-C21-O21
59	BA	1643	TAC	C1-C2-C21-N21
59	BA	1643	TAC	C3-C4-N4-C42
59	BA	1643	TAC	C3-C4-N4-C43
59	BA	1643	TAC	C41-C4-N4-C42
59	BA	1644	TAC	C1-C2-C21-O21
59	BA	1644	TAC	C1-C2-C21-N21
59	BA	1644	TAC	C3-C4-N4-C43
59	BA	1644	TAC	C41-C4-N4-C42
65	DA	3202	1PE	OH4-C13-C23-OH3
65	DA	3202	1PE	OH5-C14-C24-OH4
56	DR	202	PG4	O2-C3-C4-O3
63	DU	101	PGE	O3-C5-C6-O4
63	DA	3186	PGE	O3-C5-C6-O4
63	DA	3203	PGE	O3-C5-C6-O4
63	DU	101	PGE	O1-C1-C2-O2
63	DA	3001	PGE	O3-C5-C6-O4
63	DA	3203	PGE	O2-C3-C4-O3
56	DQ	202	PG4	O1-C1-C2-O2
56	DS	202	PG4	O1-C1-C2-O2
63	DA	3214	PGE	O3-C5-C6-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
64	DA	3224	SPD	C4-C5-N6-C7
63	DA	3186	PGE	O1-C1-C2-O2
64	DA	3206	SPD	C8-C7-N6-C5
64	DA	3183	SPD	C2-C3-C4-C5
56	DS	202	PG4	O4-C7-C8-O5
61	D1	103	PEG	O2-C3-C4-O4
61	DA	3226	PEG	O1-C1-C2-O2
65	DA	3202	1PE	OH2-C12-C22-OH3
63	DA	3225	PGE	O2-C3-C4-O3
62	DA	3197	EDO	O1-C1-C2-O2
63	DA	3225	PGE	O3-C5-C6-O4
58	AA	1675	PUT	C1-C2-C3-C4
58	DA	3223	PUT	C1-C2-C3-C4
56	DA	3193	PG4	O3-C5-C6-O4
56	DQ	202	PG4	O2-C3-C4-O3
64	DA	3187	SPD	C2-C3-C4-C5
61	DP	201	PEG	O1-C1-C2-O2
61	DA	3200	PEG	C1-C2-O2-C3
65	DA	3185	1PE	C24-C14-OH5-C25
61	DP	201	PEG	C4-C3-O2-C2
56	DA	3216	PG4	C3-C4-O3-C5
56	DR	202	PG4	C4-C3-O2-C2
63	DA	3203	PGE	C3-C4-O3-C5
56	DA	3216	PG4	C1-C2-O2-C3
61	DA	3226	PEG	C4-C3-O2-C2
65	DA	3202	1PE	C12-C22-OH3-C23
61	DA	3199	PEG	C4-C3-O2-C2
56	DA	3193	PG4	C6-C5-O3-C4
56	DS	202	PG4	C5-C6-O4-C7
56	DA	3193	PG4	C4-C3-O2-C2
63	DA	3203	PGE	C4-C3-O2-C2
63	D1	102	PGE	C4-C3-O2-C2
56	DA	3193	PG4	O1-C1-C2-O2
65	DA	3185	1PE	C12-C22-OH3-C23
64	DA	3206	SPD	C4-C5-N6-C7
61	DA	3218	PEG	C1-C2-O2-C3
61	DA	3226	PEG	C1-C2-O2-C3
63	DA	3001	PGE	C3-C4-O3-C5
65	DA	3185	1PE	C13-C23-OH3-C22
61	D3	101	PEG	C1-C2-O2-C3
61	DA	3200	PEG	C4-C3-O2-C2
63	DA	3225	PGE	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
63	D1	102	PGE	C3-C4-O3-C5
57	DN	201	MPD	O2-C2-C3-C4
57	DT	201	MPD	O2-C2-C3-C4
57	DA	3204	MPD	O2-C2-C3-C4
56	DR	202	PG4	C6-C5-O3-C4
64	DA	3224	SPD	C8-C7-N6-C5
57	DE	302	MPD	C2-C3-C4-O4
57	DA	3192	MPD	C2-C3-C4-O4
63	DU	101	PGE	C6-C5-O3-C4
63	DA	3214	PGE	C4-C3-O2-C2
63	D1	102	PGE	O1-C1-C2-O2
65	DA	3202	1PE	OH7-C16-C26-OH6
57	DT	201	MPD	C1-C2-C3-C4
57	DT	201	MPD	CM-C2-C3-C4
57	DA	3207	MPD	C1-C2-C3-C4
59	AA	1680	TAC	C3-C4-N4-C43
59	AA	1681	TAC	C3-C4-N4-C43
59	BA	1643	TAC	C41-C4-N4-C43
59	BA	1644	TAC	C3-C2-C21-N21
63	DA	3217	PGE	C1-C2-O2-C3
59	BA	1644	TAC	C3-C2-C21-O21
56	AA	1670	PG4	O1-C1-C2-O2
56	AA	1670	PG4	C4-C3-O2-C2
57	DE	301	MPD	C2-C3-C4-C5
57	DN	201	MPD	C2-C3-C4-C5
57	DT	202	MPD	C2-C3-C4-C5
57	DA	3190	MPD	C2-C3-C4-C5
57	DA	3204	MPD	C2-C3-C4-C5
57	DA	3207	MPD	C2-C3-C4-C5
59	AA	1681	TAC	C1-C2-C21-N21
61	AL	201	PEG	C4-C3-O2-C2
65	DA	3185	1PE	C16-C26-OH6-C15
65	DA	3202	1PE	C23-C13-OH4-C24
61	AL	201	PEG	C1-C2-O2-C3
63	DS	201	PGE	C6-C5-O3-C4
58	DA	3212	PUT	C1-C2-C3-C4
56	DS	202	PG4	C1-C2-O2-C3
64	DA	3224	SPD	C7-C8-C9-N10
63	DA	3001	PGE	C4-C3-O2-C2
63	DA	3217	PGE	C4-C3-O2-C2
63	DA	3001	PGE	C1-C2-O2-C3
56	DA	3216	PG4	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
63	D1	102	PGE	O2-C3-C4-O3
61	DQ	201	PEG	C1-C2-O2-C3
61	DP	201	PEG	C1-C2-O2-C3
64	DA	3187	SPD	N6-C7-C8-C9
62	DA	3002	EDO	O1-C1-C2-O2
61	DL	201	PEG	O1-C1-C2-O2
56	DA	3193	PG4	C3-C4-O3-C5
63	DA	3225	PGE	O1-C1-C2-O2
63	DA	3225	PGE	C3-C4-O3-C5
62	DA	3003	EDO	O1-C1-C2-O2
62	DA	3208	EDO	O1-C1-C2-O2
56	DA	3216	PG4	O4-C7-C8-O5
63	DA	3214	PGE	O2-C3-C4-O3
63	D1	102	PGE	C1-C2-O2-C3
63	DS	201	PGE	C1-C2-O2-C3
56	AA	1670	PG4	C1-C2-O2-C3
65	DA	3185	1PE	OH4-C13-C23-OH3
65	DA	3202	1PE	C14-C24-OH4-C13
57	AA	1671	MPD	O2-C2-C3-C4
57	DK	201	MPD	O2-C2-C3-C4
57	DT	202	MPD	O2-C2-C3-C4
56	AA	1670	PG4	C8-C7-O4-C6
57	DE	301	MPD	C2-C3-C4-O4
57	DK	201	MPD	C2-C3-C4-O4
57	DN	201	MPD	C2-C3-C4-O4
57	DT	202	MPD	C2-C3-C4-O4
57	DA	3204	MPD	C2-C3-C4-O4
61	D3	101	PEG	O1-C1-C2-O2
57	AA	1676	MPD	C1-C2-C3-C4
57	DE	301	MPD	C1-C2-C3-C4
57	DE	302	MPD	C1-C2-C3-C4
57	DK	201	MPD	C1-C2-C3-C4
57	DA	3192	MPD	CM-C2-C3-C4
57	DA	3204	MPD	CM-C2-C3-C4
57	DA	3207	MPD	CM-C2-C3-C4
59	BA	1643	TAC	C3-C2-C21-N21
56	DA	3193	PG4	O2-C3-C4-O3
56	DQ	202	PG4	C5-C6-O4-C7
59	BA	1643	TAC	C3-C2-C21-O21
56	DR	202	PG4	O3-C5-C6-O4
61	DA	3218	PEG	O1-C1-C2-O2
56	DR	202	PG4	C8-C7-O4-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	DB	212	EDO	O1-C1-C2-O2
56	DA	3193	PG4	C1-C2-O2-C3

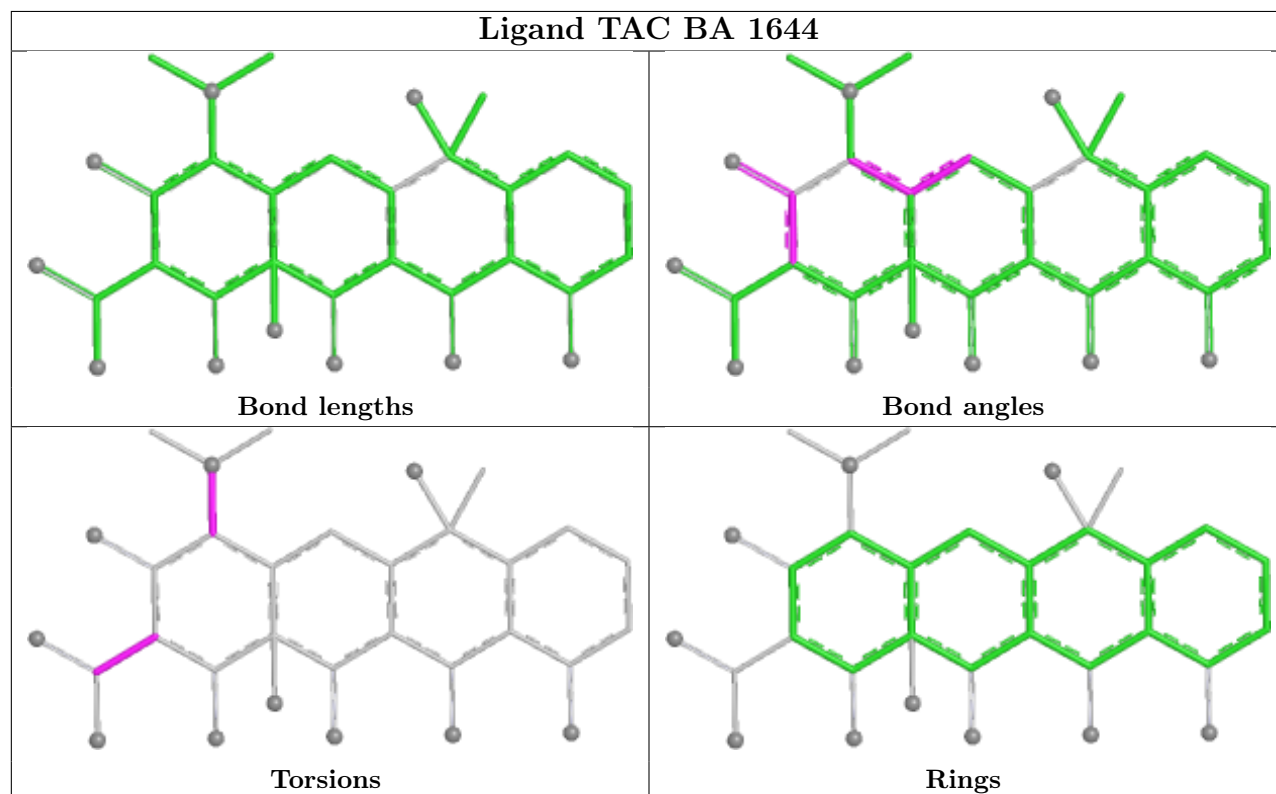
There are no ring outliers.

27 monomers are involved in 46 short contacts:

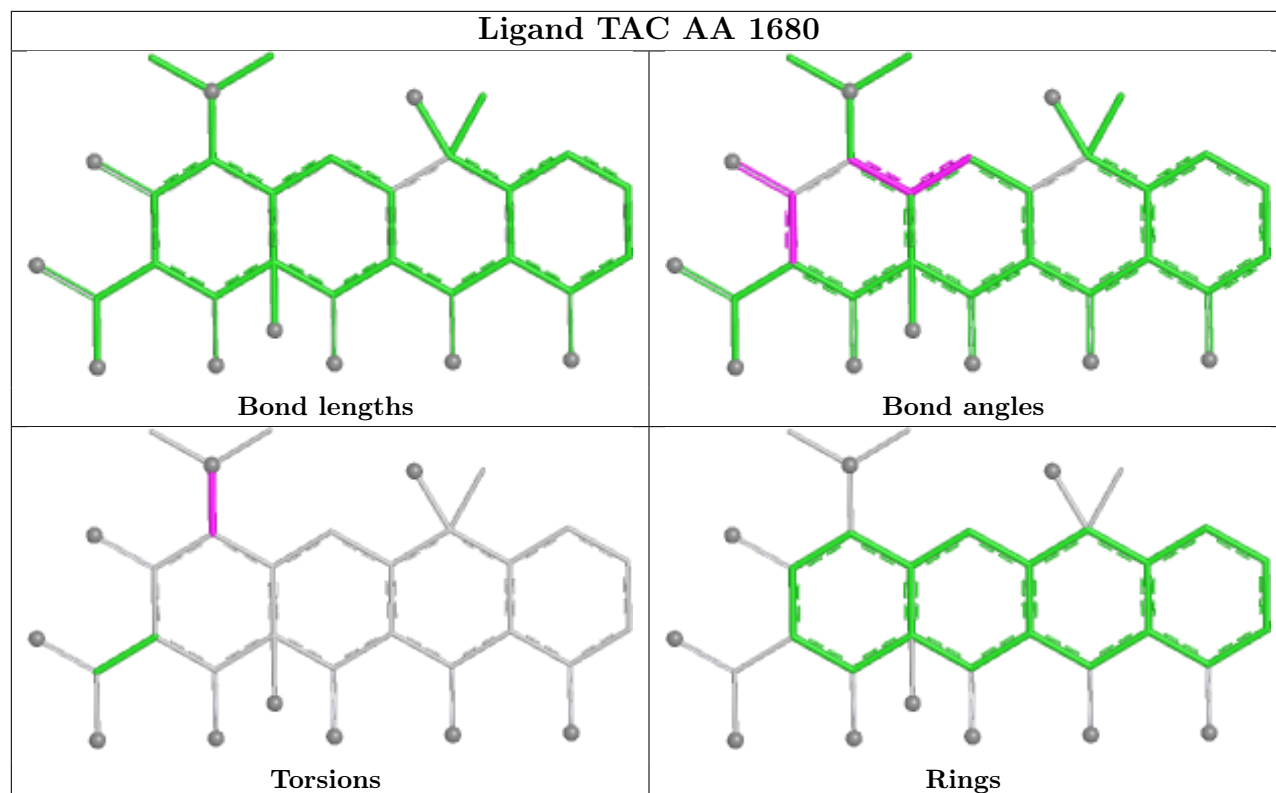
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	1642	PG4	1	0
56	DA	3216	PG4	1	0
57	AA	1676	MPD	3	0
56	DS	202	PG4	3	0
57	DN	201	MPD	1	0
63	DA	3225	PGE	2	0
56	DR	202	PG4	5	0
58	DA	3195	PUT	3	0
56	DA	3193	PG4	2	0
58	DA	3222	PUT	3	0
62	DA	3198	EDO	1	0
68	DA	3220	TRS	1	0
64	DA	3224	SPD	2	0
57	DA	3207	MPD	1	0
58	DA	3189	PUT	1	0
63	DA	3214	PGE	1	0
63	DA	3001	PGE	1	0
57	DA	3204	MPD	1	0
61	D1	103	PEG	1	0
65	DA	3202	1PE	1	0
57	DA	3192	MPD	1	0
63	DS	201	PGE	1	0
63	DU	101	PGE	3	0
59	AA	1681	TAC	2	0
56	AA	1670	PG4	1	0
61	DP	201	PEG	1	0
63	D1	102	PGE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

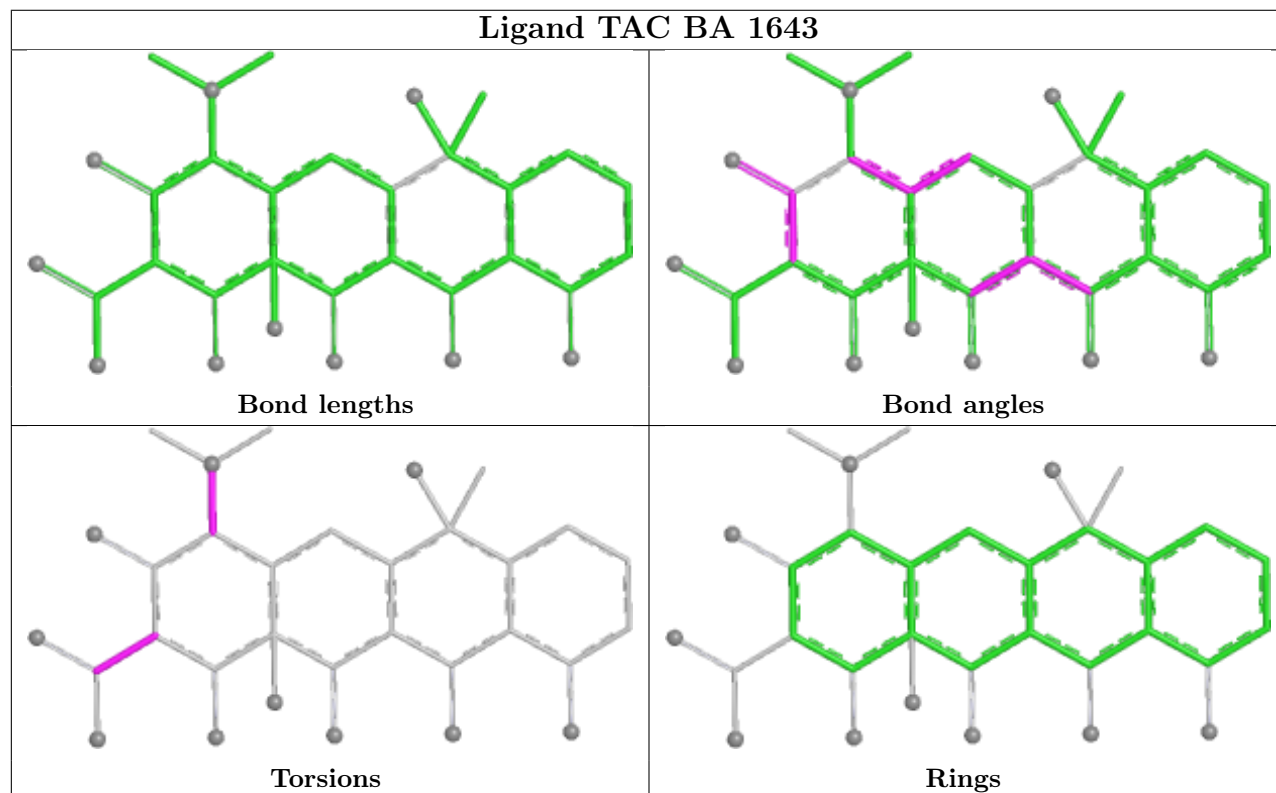
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

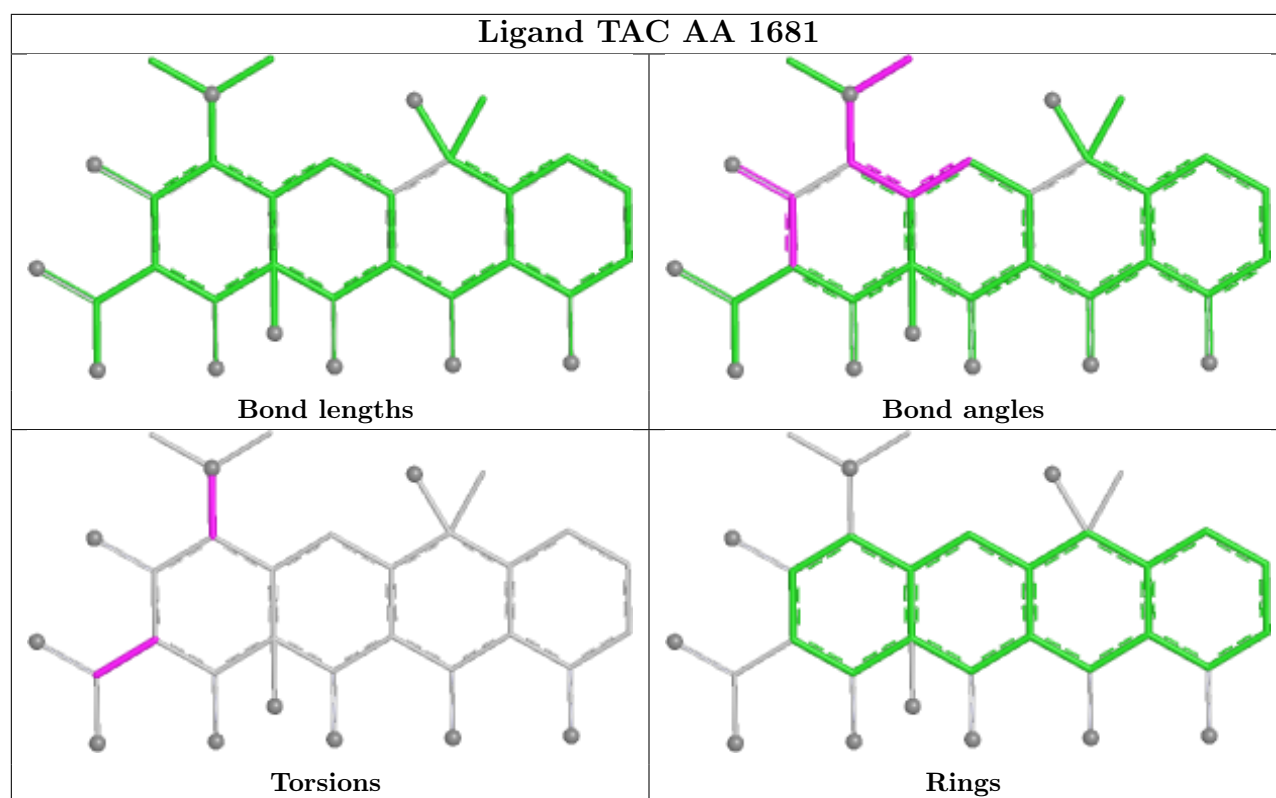


Ligand TAC AA 1680



Ligand TAC BA 1643





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.16	86 (5%) 30 15	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.63	128 (8%) 17 9	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.53	10 (4%) 38 20	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.88	24 (10%) 11 6	89, 139, 197, 228	0
3	AC	206/206 (100%)	0.26	5 (2%) 59 36	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.78	19 (9%) 14 8	90, 138, 170, 184	0
4	AD	205/205 (100%)	0.21	2 (0%) 79 59	63, 92, 129, 160	0
4	BD	205/205 (100%)	0.01	1 (0%) 87 72	53, 77, 106, 132	0
5	AE	155/155 (100%)	0.04	1 (0%) 85 69	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.60	7 (4%) 36 19	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.32	4 (3%) 44 24	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.55	6 (6%) 27 14	77, 117, 140, 153	0
7	AG	151/151 (100%)	1.27	26 (17%) 4 3	95, 136, 160, 174	0
7	BG	151/151 (100%)	1.28	30 (19%) 3 2	136, 196, 213, 220	0
8	AH	129/129 (100%)	0.17	3 (2%) 61 38	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.64	6 (4%) 36 19	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.28	22 (17%) 4 3	74, 135, 164, 171	0
9	BI	127/127 (100%)	1.59	37 (29%) 1 1	133, 164, 201, 210	0
10	AJ	99/99 (100%)	1.09	12 (12%) 8 5	83, 118, 141, 147	0
10	BJ	98/99 (98%)	1.84	38 (38%) 1 1	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.42	4 (3%) 48 27	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.65	10 (8%) 16 8	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.02	3 (2%) 58 35	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.88	16 (13%) 7 4	65, 86, 114, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.56	31 (27%) 1 1	108, 130, 165, 171	0
13	BM	114/114 (100%)	1.29	17 (14%) 5 3	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.55	28 (28%) 1 1	77, 117, 178, 184	0
14	BN	100/100 (100%)	1.68	33 (33%) 1 1	124, 178, 216, 222	0
15	AO	88/88 (100%)	0.20	2 (2%) 61 38	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.56	3 (3%) 48 27	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.44	2 (2%) 59 36	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.44	19 (23%) 2 1	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.23	1 (1%) 75 53	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.16	7 (8%) 15 8	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.32	2 (3%) 46 26	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.52	5 (9%) 15 8	65, 86, 129, 168	0
19	AS	79/79 (100%)	1.64	25 (31%) 1 1	114, 135, 155, 163	0
19	BS	79/79 (100%)	1.45	18 (22%) 2 1	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.41	4 (4%) 36 19	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.58	20 (23%) 2 1	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.50	3 (5%) 31 16	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.57	3 (5%) 31 16	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.90	25 (44%) 0 1	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.62	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	1.88	20 (40%) 1 1	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.09	1 (1%) 65 41	46, 60, 87, 104	0
24	C3	46/46 (100%)	2.37	30 (65%) 0 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.47	1 (2%) 62 39	23, 31, 48, 112	0
25	C4	64/64 (100%)	2.92	51 (79%) 0 0	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.54	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.81	14 (36%) 1 1	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.35	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	1.25	13 (22%) 2 1	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.49	0 100 100	21, 29, 53, 80	2 (3%)
28	CB	118/120 (98%)	0.69	4 (3%) 48 27	102, 170, 229, 238	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.71	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.96	50 (18%) 3 2	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.39	3 (1%) 78 57	22, 49, 76, 92	0
30	CD	208/209 (99%)	1.13	31 (14%) 5 3	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.59	1 (0%) 87 72	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	1.02	343 (11%) 9 5	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.58	60 (29%) 1 1	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.40	0 100 100	19, 50, 96, 132	0
33	CF	177/177 (100%)	1.01	17 (9%) 13 7	193, 211, 219, 227	0
33	DF	177/177 (100%)	0.09	1 (0%) 85 69	44, 75, 117, 142	0
34	CG	176/176 (100%)	0.81	8 (4%) 38 20	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.08	1 (0%) 85 69	38, 66, 97, 123	0
35	CH	149/149 (100%)	0.69	7 (4%) 36 19	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.71	5 (3%) 48 27	55, 142, 179, 198	0
36	CJ	134/134 (100%)	1.60	41 (30%) 1 1	235, 251, 263, 270	0
36	DJ	134/134 (100%)	1.75	45 (33%) 1 1	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.97	13 (9%) 14 8	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.67	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	1.02	12 (9%) 13 7	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.59	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	1.67	52 (36%) 1 1	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.37	1 (0%) 84 66	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.81	10 (7%) 20 10	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.65	0 100 100	13, 34, 63, 95	1 (0%)
41	CO	120/125 (96%)	1.70	38 (31%) 1 1	94, 117, 139, 180	0
41	DO	125/125 (100%)	-0.54	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	0.89	16 (13%) 6 4	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.29	1 (0%) 81 61	34, 52, 82, 94	0
43	CQ	114/114 (100%)	1.13	13 (11%) 10 6	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.39	1 (0%) 81 61	26, 43, 75, 116	0
44	CR	117/117 (100%)	1.37	31 (26%) 1 1	81, 103, 125, 141	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DR	117/117 (100%)	-0.74	0 100 100	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.40	27 (26%) 1 1	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.57	2 (1%) 66 43	15, 39, 68, 94	0
46	CT	110/110 (100%)	1.74	34 (30%) 1 1	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.58	1 (0%) 81 61	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.84	35 (37%) 1 1	124, 146, 173, 182	0
47	DU	93/93 (100%)	0.09	5 (5%) 31 16	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.14	55 (53%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.18	1 (0%) 79 59	36, 56, 101, 131	0
49	CW	94/94 (100%)	0.78	7 (7%) 20 10	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.36	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.22	12 (16%) 5 3	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.41	0 100 100	16, 36, 62, 104	1 (1%)
51	CY	77/77 (100%)	1.48	21 (27%) 1 1	78, 113, 143, 160	0
51	DY	77/77 (100%)	-0.30	1 (1%) 75 53	24, 50, 85, 112	0
52	CZ	62/62 (100%)	1.69	19 (30%) 1 1	123, 162, 179, 190	0
52	DZ	62/62 (100%)	0.11	2 (3%) 50 29	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.40	30 (22%) 2 1	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.73	102 (3%) 46 26	15, 39, 206, 298	11 (0%)
All	All	20632/20745 (99%)	0.46	2037 (9%) 13 7	10, 100, 227, 298	16 (0%)

All (2037) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	11.1
1	AA	121	U	9.2
10	BJ	74	VAL	8.5
54	DA	1731	G	7.9
54	DA	2120	G	7.4
31	CA	2172	U	7.4
9	BI	68	LYS	6.9
30	CD	126	ASN	6.8
7	BG	4	ARG	6.7
31	CA	331	C	6.6
9	BI	16	ALA	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	BJ	41	PRO	6.5
12	AL	124	ALA	6.5
31	CA	2402	U	6.4
14	AN	21	PHE	6.4
39	CM	81	ASP	6.3
20	BT	4	ILE	6.3
47	CU	43	ILE	6.3
25	C4	36	LYS	6.2
48	CV	31	SER	6.2
36	DJ	54	PRO	6.2
25	C4	28	ASN	6.1
47	CU	36	LYS	6.1
21	BU	57	ALA	6.1
17	BQ	70	THR	6.0
7	AG	4	ARG	6.0
9	BI	124	ARG	6.0
1	AA	1030	U	5.9
10	BJ	8	ILE	5.9
22	C1	2	ALA	5.9
19	BS	12	ASP	5.9
7	BG	5	ARG	5.9
23	C2	24	THR	5.9
10	BJ	75	ASP	5.8
48	CV	80	ALA	5.8
54	DA	2172	U	5.8
32	CE	104	ALA	5.7
5	BE	91	GLY	5.6
36	CJ	23	PRO	5.6
25	C4	37	ALA	5.6
9	AI	20	PHE	5.6
1	BA	121	U	5.6
20	BT	5	LYS	5.6
37	CK	81	ILE	5.6
41	CO	46	ARG	5.5
18	BR	20	GLU	5.4
1	BA	632	U	5.4
32	CE	32	VAL	5.4
36	CJ	13	VAL	5.3
53	DI	38	MET	5.3
1	BA	1242	G	5.3
1	BA	983	A	5.3
1	AA	1019	A	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	DA	2886[A]	A	5.2
45	CS	78	ARG	5.2
36	DJ	135	SER	5.2
31	CA	12	U	5.2
37	CK	111	LYS	5.1
1	AA	1364	U	5.1
31	CA	2800	A	5.1
46	CT	82	MET	5.1
25	C4	41	LYS	5.1
41	CO	25	ALA	5.1
25	C4	40	ARG	5.0
1	AA	984	C	5.0
24	C3	24	THR	5.0
32	CE	33	VAL	5.0
9	BI	116	VAL	5.0
29	CC	242	LYS	5.0
48	CV	13	VAL	5.0
1	AA	962	C	5.0
52	CZ	45	GLN	5.0
31	CA	2383	G	4.9
1	BA	307	C	4.9
45	CS	73	LYS	4.9
13	BM	96	PRO	4.9
21	AU	57	ALA	4.9
25	C4	60	ALA	4.9
1	BA	1243	C	4.9
9	BI	119	ARG	4.8
46	CT	43	ALA	4.8
46	CT	97	LEU	4.8
54	DA	1087	G	4.8
24	D3	46	LYS	4.8
1	AA	1148	U	4.8
47	DU	70	HIS	4.8
7	AG	109	ARG	4.8
43	DQ	2	SER	4.8
44	CR	9	ILE	4.7
9	BI	128	SER	4.7
48	CV	35	ILE	4.7
39	CM	14	LYS	4.7
1	AA	1127	G	4.7
31	CA	1984	G	4.7
13	AM	105	ASN	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AA	959	A	4.7
23	C2	22	THR	4.6
18	BR	51	TYR	4.6
48	CV	5	ILE	4.6
1	BA	1305	G	4.6
31	CA	329	G	4.6
54	DA	2141	G	4.6
7	BG	62	PHE	4.6
19	AS	71	LEU	4.6
44	CR	8	VAL	4.6
13	AM	30	SER	4.6
31	CA	1068	G	4.6
31	CA	2174	C	4.6
12	BL	70	GLU	4.6
10	AJ	75	ASP	4.5
53	DI	126	LEU	4.5
1	AA	963	G	4.5
32	CE	73	ILE	4.5
20	BT	6	SER	4.5
20	BT	13	GLN	4.5
2	AB	30	PHE	4.5
24	C3	23	ALA	4.5
54	DA	2152	G	4.5
48	CV	30	SER	4.5
7	AG	32	VAL	4.5
27	C0	56	LYS	4.5
48	CV	36	VAL	4.5
25	C4	29	LEU	4.5
10	BJ	39	PRO	4.5
1	BA	4	U	4.4
9	BI	125	PRO	4.4
6	BF	100	SER	4.4
10	BJ	76	ILE	4.4
41	CO	23	ASN	4.4
44	CR	28	ARG	4.4
31	CA	931	U	4.4
13	AM	19	LEU	4.4
36	DJ	138	LEU	4.4
38	CL	122	VAL	4.4
54	DA	1090	A	4.4
1	AA	1286	U	4.4
46	CT	84	ARG	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DJ	13	VAL	4.4
48	CV	3	ALA	4.4
53	DI	93	ALA	4.4
1	AA	1128	C	4.4
31	CA	183	C	4.4
31	CA	776	G	4.3
48	CV	39	ILE	4.3
36	DJ	12	GLN	4.3
54	DA	1089	A	4.3
36	DJ	24	VAL	4.3
38	CL	35	VAL	4.3
24	C3	42	LEU	4.3
1	BA	108	G	4.3
1	BA	306	A	4.3
14	BN	47	LYS	4.3
10	BJ	73	LEU	4.3
25	C4	39	LYS	4.3
33	CF	156	ILE	4.3
31	CA	1238	G	4.3
16	BP	57	ILE	4.3
1	BA	211	G	4.2
1	BA	1364	U	4.2
54	DA	1847	A	4.2
13	AM	24	GLY	4.2
53	DI	36	ASP	4.2
1	BA	201	G	4.2
31	CA	2666	C	4.2
11	BK	14	LYS	4.2
32	CE	178	VAL	4.2
32	CE	164	LEU	4.2
31	CA	2690	U	4.2
36	CJ	11	LEU	4.2
45	DS	103	ALA	4.2
53	DI	83	ALA	4.2
7	AG	106	GLU	4.2
1	BA	1201	A	4.2
53	DI	131	THR	4.2
54	DA	1091	G	4.2
19	BS	37	ARG	4.2
13	BM	89	LEU	4.1
13	BM	106	ALA	4.1
2	BB	132	LYS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	97	LYS	4.1
29	CC	30	PHE	4.1
1	BA	212	G	4.1
19	BS	76	PRO	4.1
16	BP	17	TYR	4.1
31	CA	332	A	4.1
22	C1	21	ALA	4.1
1	BA	1241	G	4.1
25	C4	57	LEU	4.1
25	C4	38	THR	4.1
13	AM	33	ILE	4.1
46	CT	85	ILE	4.1
25	C4	25	LYS	4.1
47	CU	33	LYS	4.1
31	CA	1215	G	4.1
54	DA	2110	G	4.1
29	CC	12	GLY	4.1
51	CY	20	HIS	4.1
46	CT	94	ASP	4.0
25	C4	61	CYS	4.0
39	CM	8	PRO	4.0
25	C4	7	VAL	4.0
54	DA	277	G	4.0
10	BJ	69	THR	4.0
19	AS	39	THR	4.0
36	CJ	76	ALA	4.0
31	CA	513	A	4.0
1	AA	961	U	4.0
44	CR	13	ARG	4.0
54	DA	1729	U	4.0
33	CF	32	GLU	4.0
31	CA	326	G	4.0
2	BB	131	LYS	4.0
22	C1	27	SER	4.0
39	CM	15	ALA	4.0
36	DJ	53	LEU	4.0
1	AA	951	G	4.0
31	CA	75	G	4.0
31	CA	327	G	4.0
31	CA	386	G	4.0
46	CT	44	ALA	4.0
10	AJ	6	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DJ	55	ILE	3.9
25	C4	3	LYS	3.9
50	CX	44	LYS	3.9
1	AA	1020	G	3.9
50	CX	54	GLY	3.9
45	CS	81	LYS	3.9
29	CC	251	GLN	3.9
19	BS	49	ILE	3.9
31	CA	515	A	3.9
41	CO	105	GLY	3.9
45	CS	82	HIS	3.9
1	AA	977	A	3.9
44	CR	11	ARG	3.9
31	CA	2363	G	3.9
36	DJ	38	PHE	3.9
9	BI	117	GLY	3.8
20	BT	69	LYS	3.8
23	C2	37	LYS	3.8
1	BA	1218	C	3.8
9	BI	126	GLN	3.8
39	DM	104	GLN	3.8
7	AG	23	LEU	3.8
36	DJ	133	ALA	3.8
2	AB	27	MET	3.8
49	CW	48	MET	3.8
53	DI	106	PHE	3.8
9	AI	129	LYS	3.8
39	CM	100	ILE	3.8
41	CO	104	ALA	3.8
52	CZ	49	ASP	3.8
1	AA	1441	A	3.8
1	AA	1240	U	3.8
36	CJ	56	PRO	3.8
31	CA	805	G	3.8
26	C5	32	LYS	3.8
48	CV	26	LYS	3.8
43	CQ	84	ILE	3.8
47	CU	61	LEU	3.8
1	BA	250	A	3.8
23	C2	23	THR	3.8
31	CA	330	A	3.8
31	CA	1104	C	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	DZ	63	ALA	3.7
35	DH	12	LEU	3.7
36	DJ	80	LEU	3.7
46	CT	46	LEU	3.7
7	AG	26	PHE	3.7
10	BJ	44	THR	3.7
46	CT	83	LYS	3.7
11	BK	84	VAL	3.7
31	CA	328	U	3.7
36	DJ	58	VAL	3.7
54	DA	1078	U	3.7
1	AA	958	A	3.7
31	CA	829	A	3.7
31	CA	1067	A	3.7
31	CA	765	C	3.7
23	C2	34	LEU	3.7
7	AG	62	PHE	3.7
9	BI	127	PHE	3.7
43	CQ	111	LYS	3.7
9	BI	121	ALA	3.7
29	CC	47	GLY	3.7
37	CK	42	ALA	3.7
24	C3	1	MET	3.7
31	CA	411	G	3.7
1	AA	1086	U	3.7
1	AA	983	A	3.7
29	CC	3	VAL	3.7
31	CA	335	C	3.7
31	CA	1547	C	3.7
14	BN	60	GLN	3.7
36	CJ	122	ILE	3.7
1	AA	1492	A	3.6
1	BA	1236	A	3.6
1	BA	1362	A	3.6
20	BT	67	ILE	3.6
32	CE	30	GLN	3.6
41	CO	9	GLN	3.6
44	CR	59	GLN	3.6
54	DA	892	A	3.6
23	C2	21	TYR	3.6
1	BA	1126	U	3.6
1	BA	1321	U	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	C1	5	GLN	3.6
1	AA	973	G	3.6
31	CA	2127	G	3.6
47	CU	62	VAL	3.6
54	DA	2153	C	3.6
14	BN	12	LYS	3.6
39	CM	61	LEU	3.6
47	CU	74	ILE	3.6
29	CC	233	GLY	3.6
44	CR	3	ARG	3.6
2	BB	187	VAL	3.6
31	CA	1216	G	3.6
31	CA	1393	A	3.6
7	AG	42	ILE	3.6
10	BJ	25	ILE	3.6
45	CS	27	ILE	3.6
1	AA	1140	C	3.6
31	CA	257	C	3.6
9	AI	117	GLY	3.6
25	C4	27	ALA	3.6
1	BA	219	U	3.6
25	C4	15	LYS	3.6
53	DI	95	LEU	3.6
8	AH	2	SER	3.6
31	CA	675	A	3.5
31	CA	1085	A	3.5
31	CA	2346	A	3.5
31	CA	2525	G	3.5
39	CM	59	ARG	3.5
29	CC	234	GLY	3.5
31	CA	1958	C	3.5
46	CT	45	VAL	3.5
3	BC	71	ALA	3.5
47	DU	1	MET	3.5
9	AI	89	GLU	3.5
43	CQ	68	GLU	3.5
43	CQ	110	ILE	3.5
19	AS	74	PHE	3.5
22	C1	11	SER	3.5
26	C5	2	LYS	3.5
48	CV	24	LYS	3.5
1	AA	994	A	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	609	A	3.5
31	CA	1084	A	3.5
54	DA	549	G	3.5
1	AA	985	C	3.5
14	AN	55	SER	3.5
48	DV	56	GLY	3.5
52	CZ	32	ALA	3.5
30	CD	23	PRO	3.5
38	CL	94	PRO	3.5
1	BA	949	A	3.5
35	DH	11	ASN	3.5
31	CA	1986	C	3.5
54	DA	1730	C	3.5
31	CA	1106	G	3.5
34	CG	175	LYS	3.5
36	CJ	12	GLN	3.5
42	CP	30	ARG	3.5
47	CU	73	ARG	3.5
29	CC	241	GLY	3.5
54	DA	2108	A	3.5
2	BB	147	SER	3.5
14	BN	96	LEU	3.5
1	BA	1302	C	3.5
32	CE	67	ARG	3.5
32	CE	175	ILE	3.5
1	AA	1018	G	3.5
54	DA	2107	G	3.5
31	CA	1105	U	3.5
48	CV	44	LYS	3.4
16	BP	27	ALA	3.4
20	BT	68	HIS	3.4
44	CR	2	ALA	3.4
7	AG	7	ILE	3.4
9	BI	14	SER	3.4
9	BI	122	ARG	3.4
25	C4	4	ILE	3.4
1	BA	1067	A	3.4
54	DA	613	A	3.4
1	BA	631	C	3.4
14	AN	97	LYS	3.4
31	CA	481	G	3.4
10	BJ	38	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	BT	66	LEU	3.4
33	CF	131	GLY	3.4
53	DI	72	LEU	3.4
24	C3	43	THR	3.4
14	BN	70	PRO	3.4
38	CL	48	PRO	3.4
48	CV	83	VAL	3.4
12	BL	124	ALA	3.4
1	BA	1049	U	3.4
36	DJ	94	ASN	3.4
3	AC	207	ILE	3.4
25	C4	43	HIS	3.4
32	CE	77	ILE	3.4
13	AM	112	PRO	3.4
1	AA	1015	G	3.4
1	BA	633	G	3.4
39	CM	80	SER	3.4
33	CF	31	VAL	3.4
2	BB	136	MET	3.4
32	CE	36	ALA	3.4
48	CV	75	ALA	3.4
1	AA	1016	A	3.4
9	BI	120	LYS	3.4
25	C4	14	PHE	3.4
11	BK	94	GLU	3.4
9	AI	119	ARG	3.4
36	CJ	24	VAL	3.4
46	CT	95	ARG	3.4
31	CA	2895	G	3.4
3	BC	155	GLY	3.4
30	CD	57	ALA	3.4
39	CM	49	GLY	3.4
14	BN	93	ILE	3.4
39	CM	84	LYS	3.4
19	BS	33	THR	3.4
31	CA	508	A	3.3
31	CA	2602	A	3.3
1	AA	1017	U	3.3
31	CA	1217	U	3.3
43	CQ	85	SER	3.3
45	DS	26	ASP	3.3
20	BT	64	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	C4	52	LYS	3.3
44	CR	22	LYS	3.3
36	CJ	55	ILE	3.3
31	CA	2410	G	3.3
54	DA	2125	G	3.3
19	AS	60	VAL	3.3
48	CV	29	LEU	3.3
50	CX	17	GLU	3.3
19	BS	35	SER	3.3
41	CO	40	LYS	3.3
54	DA	654	A	3.3
41	CO	24	MET	3.3
45	CS	49	ILE	3.3
1	BA	982	U	3.3
19	AS	3	ARG	3.3
25	C4	55	LEU	3.3
1	AA	971	G	3.3
1	AA	1305	G	3.3
8	BH	2	SER	3.3
20	BT	63	ALA	3.3
31	CA	2067	G	3.3
51	CY	64	ILE	3.3
20	BT	36	TYR	3.3
1	BA	1219	A	3.3
31	CA	514	A	3.3
35	CH	27	ARG	3.3
39	CM	30	THR	3.3
39	CM	35	HIS	3.3
50	CX	55	ARG	3.3
54	DA	1061	U	3.3
31	CA	76	C	3.3
31	CA	105	C	3.3
32	CE	143	LEU	3.3
33	CF	152	LEU	3.3
54	DA	2174	C	3.3
29	CC	213	TRP	3.3
24	C3	40	ALA	3.3
25	C4	65	ALA	3.3
39	CM	51	GLU	3.3
13	BM	86	TYR	3.3
25	C4	2	PRO	3.3
36	CJ	74	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	CS	86	GLN	3.3
23	C2	10	LYS	3.3
44	CR	4	VAL	3.3
54	DA	1077	A	3.3
54	DA	1084	A	3.3
1	BA	470	C	3.3
54	DA	2175	C	3.3
26	C5	21	GLY	3.3
39	CM	11	GLY	3.3
12	BL	86	ARG	3.2
32	CE	93	SER	3.2
10	BJ	102	LEU	3.2
7	BG	35	LYS	3.2
14	AN	71	HIS	3.2
10	BJ	26	VAL	3.2
36	CJ	140	VAL	3.2
36	DJ	118	THR	3.2
11	AK	110	ILE	3.2
1	AA	1353	G	3.2
26	C5	38	GLY	3.2
39	CM	53	GLY	3.2
52	CZ	17	GLU	3.2
54	DA	2151	U	3.2
19	AS	55	ARG	3.2
44	CR	33	ARG	3.2
32	CE	75	SER	3.2
36	CJ	79	LEU	3.2
51	CY	49	LEU	3.2
53	DI	24	SER	3.2
53	DI	96	PHE	3.2
25	C4	54	ASP	3.2
46	CT	96	ILE	3.2
30	CD	192	ALA	3.2
38	CL	33	ALA	3.2
30	CD	10	GLY	3.2
41	CO	43	GLU	3.2
42	CP	7	ARG	3.2
25	C4	33	LEU	3.2
32	CE	101	TYR	3.2
52	CZ	57	LEU	3.2
31	CA	767	U	3.2
54	DA	2109	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	C1	3	VAL	3.2
31	CA	1381	G	3.2
1	AA	1031	C	3.2
36	DJ	96	ASP	3.2
47	CU	35	ALA	3.2
45	CS	88	GLY	3.2
29	CC	236	GLU	3.2
22	C1	12	LYS	3.2
26	C5	10	LEU	3.2
36	CJ	80	LEU	3.2
39	CM	19	LEU	3.2
7	BG	43	VAL	3.2
10	AJ	74	VAL	3.2
33	CF	132	VAL	3.2
53	DI	33	VAL	3.2
1	BA	1235	U	3.2
14	AN	32	SER	3.2
19	AS	56	GLN	3.2
39	CM	101	ILE	3.2
41	CO	22	ARG	3.2
46	CT	100	THR	3.2
22	C1	24	ALA	3.2
31	CA	2070	A	3.2
25	C4	35	LYS	3.2
30	CD	8	LYS	3.2
31	CA	26	G	3.2
31	CA	68	G	3.2
2	BB	135	LEU	3.2
19	AS	5	LEU	3.2
32	CE	134	LEU	3.2
32	CE	200	LEU	3.2
25	C4	46	PRO	3.2
36	CJ	54	PRO	3.2
16	BP	42	ILE	3.2
24	C3	35	ARG	3.2
39	CM	72	ALA	3.2
1	AA	1049	U	3.1
14	AN	18	ASP	3.1
14	AN	54	ASP	3.1
1	AA	1331	G	3.1
31	CA	1210	G	3.1
31	CA	2364	C	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	CD	128	ARG	3.1
36	DJ	129	ILE	3.1
2	AB	132	LYS	3.1
32	CE	135	ALA	3.1
44	CR	38	ALA	3.1
29	CC	202	LEU	3.1
9	AI	125	PRO	3.1
24	C3	13	ASN	3.1
45	CS	83	TYR	3.1
46	CT	99	ARG	3.1
1	AA	974	A	3.1
22	C1	15	MET	3.1
31	CA	1548	A	3.1
31	CA	2173	A	3.1
54	DA	1103	A	3.1
14	AN	12	LYS	3.1
54	DA	2150	C	3.1
19	AS	9	PRO	3.1
10	BJ	40	ILE	3.1
17	BQ	5	ILE	3.1
36	DJ	117	MET	3.1
48	CV	17	LYS	3.1
47	CU	93	LEU	3.1
51	CY	30	LEU	3.1
3	BC	192	THR	3.1
14	AN	50	THR	3.1
25	C4	56	GLY	3.1
31	CA	2126	A	3.1
33	CF	93	GLY	3.1
32	CE	72	SER	3.1
13	AM	25	VAL	3.1
16	AP	39	PHE	3.1
19	AS	73	GLU	3.1
30	CD	200	ASP	3.1
54	DA	1172	C	3.1
17	AQ	53	CYS	3.1
27	C0	18	PRO	3.1
40	CN	69	PRO	3.1
1	AA	933	G	3.1
1	AA	1139	G	3.1
1	BA	202	G	3.1
28	CB	98	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	2677	G	3.1
2	BB	134	ALA	3.1
36	CJ	14	ALA	3.1
32	CE	153	LEU	3.1
29	CC	212	ARG	3.1
19	AS	58	VAL	3.1
22	C1	18	SER	3.1
29	CC	245	VAL	3.1
52	CZ	40	SER	3.1
1	BA	325	A	3.1
13	BM	27	LYS	3.1
39	CM	10	GLU	3.1
30	CD	131	ASP	3.1
31	CA	53	A	3.1
31	CA	2406	A	3.1
47	CU	19	LYS	3.1
7	BG	7	ILE	3.1
9	AI	21	ILE	3.1
18	BR	21	ILE	3.1
19	AS	49	ILE	3.1
39	CM	77	ILE	3.1
31	CA	318	C	3.0
31	CA	1764	C	3.0
30	CD	132	ALA	3.0
41	CO	11	ASN	3.0
1	BA	1244	G	3.0
7	AG	8	GLY	3.0
27	C0	15	GLY	3.0
31	CA	325	G	3.0
31	CA	2409	G	3.0
54	DA	2140	G	3.0
54	DA	2885[A]	G	3.0
26	C5	3	VAL	3.0
16	BP	46	LYS	3.0
23	C2	38	LYS	3.0
39	CM	29	LYS	3.0
29	CC	38	SER	3.0
32	CE	70	SER	3.0
38	CL	28	SER	3.0
25	C4	63	PRO	3.0
24	C3	10	LEU	3.0
41	CO	28	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	1145	A	3.0
31	CA	1214	A	3.0
51	CY	28	ARG	3.0
1	AA	1149	C	3.0
39	CM	16	GLY	3.0
48	CV	32	GLY	3.0
25	C4	47	LYS	3.0
33	CF	130	MET	3.0
41	CO	1	MET	3.0
1	BA	1125	U	3.0
54	DA	1101	U	3.0
31	CA	2444	G	3.0
13	AM	95	LEU	3.0
36	CJ	106	LEU	3.0
36	DJ	79	LEU	3.0
52	CZ	18	LEU	3.0
7	BG	39	ALA	3.0
20	BT	72	ALA	3.0
52	CZ	61	ALA	3.0
46	CT	11	ARG	3.0
41	CO	3	HIS	3.0
24	C3	11	LYS	3.0
27	C0	9	GLN	3.0
1	AA	1306	A	3.0
1	BA	196	A	3.0
9	AI	19	VAL	3.0
31	CA	2665	A	3.0
48	CV	67	VAL	3.0
1	BA	222	C	3.0
3	BC	196	ILE	3.0
9	AI	28	ILE	3.0
32	CE	119	ILE	3.0
51	CY	56	MET	3.0
43	CQ	95	ALA	3.0
1	BA	208	U	3.0
10	AJ	60	ASP	3.0
31	CA	150	U	3.0
31	CA	1325	U	3.0
14	BN	7	LYS	3.0
25	C4	19	LYS	3.0
26	C5	18	LYS	3.0
30	CD	160	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	CR	5	LYS	3.0
41	CO	26	GLY	3.0
31	CA	2627	G	3.0
41	CO	21	PHE	3.0
48	CV	12	ILE	3.0
1	AA	306	A	3.0
13	AM	96	PRO	3.0
19	BS	71	LEU	3.0
36	DJ	106	LEU	3.0
54	DA	2154	A	3.0
24	C3	14	ARG	3.0
18	AR	51	TYR	3.0
51	CY	54	LYS	3.0
36	DJ	9	VAL	3.0
48	CV	49	VAL	3.0
30	CD	156	PHE	3.0
26	C5	23	ILE	3.0
24	C3	31	LEU	2.9
1	BA	1304	G	2.9
31	CA	1324	G	2.9
54	DA	283	G	2.9
54	DA	2127	G	2.9
24	C3	46	LYS	2.9
39	CM	70	LYS	2.9
46	CT	81	SER	2.9
31	CA	1103	A	2.9
3	BC	158	GLY	2.9
36	CJ	78	VAL	2.9
8	BH	90	ASP	2.9
39	CM	38	GLN	2.9
1	AA	1281	C	2.9
36	CJ	129	ILE	2.9
2	BB	129	LEU	2.9
24	C3	4	THR	2.9
31	CA	2629	U	2.9
39	CM	48	ARG	2.9
34	CG	172	LYS	2.9
36	DJ	10	LYS	2.9
50	CX	78	LYS	2.9
9	BI	17	ALA	2.9
14	AN	22	ALA	2.9
46	CT	20	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	CU	34	VAL	2.9
48	CV	59	VAL	2.9
53	DI	90	GLY	2.9
31	CA	1026	G	2.9
54	DA	879	G	2.9
19	BS	11	ILE	2.9
1	AA	1014	A	2.9
13	AM	101	ARG	2.9
15	BO	58	ARG	2.9
31	CA	2062	A	2.9
31	CA	2358	A	2.9
36	DJ	11	LEU	2.9
45	CS	80	ARG	2.9
7	AG	38	THR	2.9
1	AA	1243	C	2.9
1	BA	948	C	2.9
2	BB	34	ALA	2.9
29	CC	61	ALA	2.9
31	CA	1518	C	2.9
53	DI	2	ALA	2.9
54	DA	1102	C	2.9
1	BA	1240	U	2.9
31	CA	2449	U	2.9
36	CJ	9	VAL	2.9
29	DC	272	SER	2.9
48	CV	20	GLY	2.9
11	BK	110	ILE	2.9
19	BS	13	LEU	2.9
25	C4	44	LEU	2.9
38	CL	66	LYS	2.9
48	CV	33	LYS	2.9
29	CC	9	THR	2.9
51	CY	48	THR	2.9
1	BA	1386	G	2.9
53	DI	40	GLU	2.9
16	BP	60	TRP	2.9
31	CA	311	A	2.9
31	CA	480	A	2.9
31	CA	482	A	2.9
14	BN	11	VAL	2.9
45	CS	72	VAL	2.9
1	BA	1317	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	1963	U	2.9
14	BN	9	ARG	2.9
13	BM	19	LEU	2.9
35	CH	35	LYS	2.9
48	CV	61	LYS	2.9
14	AN	15	ALA	2.9
25	C4	6	THR	2.9
48	CV	77	THR	2.9
51	CY	31	PRO	2.9
9	BI	111	VAL	2.9
13	AM	94	GLY	2.9
13	AM	109	ARG	2.9
41	CO	4	ARG	2.9
1	BA	630	A	2.9
9	BI	100	LYS	2.9
10	AJ	25	ILE	2.9
10	BJ	59	LYS	2.9
10	BJ	100	ILE	2.9
14	AN	46	LEU	2.9
22	C1	55	ILE	2.9
31	CA	474	G	2.9
31	CA	830	G	2.9
31	CA	1205	A	2.9
31	CA	1321	A	2.9
54	DA	1085	A	2.9
1	AA	4	U	2.8
31	CA	433	C	2.8
31	CA	1606	C	2.8
31	CA	1732	C	2.8
31	CA	2149	U	2.8
31	CA	2245	U	2.8
32	CE	90	GLN	2.8
41	CO	27	SER	2.8
39	CM	75	ALA	2.8
3	BC	26	THR	2.8
27	C0	10	THR	2.8
52	CZ	24	GLU	2.8
2	BB	163	VAL	2.8
9	BI	67	VAL	2.8
25	C4	58	VAL	2.8
12	BL	18	LYS	2.8
10	BJ	52	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	CD	118	PHE	2.8
50	CX	52	GLY	2.8
26	C5	26	ILE	2.8
45	CS	7	SER	2.8
47	CU	72	GLN	2.8
53	DI	111	ALA	2.8
1	BA	1086	U	2.8
31	CA	1779	U	2.8
47	CU	14	PRO	2.8
54	DA	884	U	2.8
1	AA	87	C	2.8
1	BA	979	C	2.8
31	CA	225	C	2.8
39	CM	106	GLU	2.8
47	DU	56	GLU	2.8
54	DA	2165	C	2.8
32	CE	78	TRP	2.8
14	AN	23	LYS	2.8
9	BI	44	ALA	2.8
14	AN	56	SER	2.8
46	CT	101	SER	2.8
10	BJ	7	ARG	2.8
44	CR	30	ARG	2.8
7	BG	38	THR	2.8
13	AM	102	THR	2.8
47	CU	47	VAL	2.8
47	CU	63	VAL	2.8
29	CC	39	LYS	2.8
42	CP	4	LYS	2.8
54	DA	2163	A	2.8
36	CJ	28	LEU	2.8
3	AC	78	GLY	2.8
13	AM	73	ILE	2.8
25	C4	59	ILE	2.8
45	CS	50	GLY	2.8
1	AA	1317	C	2.8
54	DA	1056	G	2.8
54	DA	1092	C	2.8
54	DA	1093	G	2.8
36	DJ	76	ALA	2.8
38	CL	3	GLN	2.8
7	BG	45	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	AU	2	PRO	2.8
22	C1	25	VAL	2.8
36	DJ	23	PRO	2.8
51	CY	35	SER	2.8
2	BB	130	THR	2.8
6	BF	39	LEU	2.8
14	BN	101	TRP	2.8
8	BH	3	MET	2.8
10	AJ	8	ILE	2.8
19	BS	66	MET	2.8
40	CN	136	MET	2.8
1	BA	974	A	2.8
54	DA	2585	U	2.8
54	DA	2602	A	2.8
22	C1	19	HIS	2.8
25	C4	26	HIS	2.8
51	DY	20	HIS	2.8
5	BE	157	ARG	2.8
19	BS	3	ARG	2.8
1	BA	634	C	2.8
1	BA	1217	C	2.8
11	BK	21	ALA	2.8
14	AN	4	GLN	2.8
31	CA	1167	C	2.8
42	CP	6	ALA	2.8
54	DA	885	C	2.8
1	AA	1244	G	2.8
29	CC	19	VAL	2.8
54	DA	2133	G	2.8
9	AI	63	LEU	2.8
9	BI	118	LEU	2.8
10	BJ	42	LEU	2.8
9	BI	69	GLY	2.7
29	CC	27	GLY	2.7
37	CK	47	HIS	2.7
3	BC	30	ALA	2.7
1	AA	1201	A	2.7
13	AM	16	VAL	2.7
14	AN	45	VAL	2.7
41	CO	29	VAL	2.7
54	DA	1080	A	2.7
41	CO	83	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	10	GLU	2.7
31	CA	2000	C	2.7
43	CQ	27	GLU	2.7
54	DA	1104	C	2.7
3	BC	159	GLY	2.7
5	BE	109	GLY	2.7
29	CC	41	GLY	2.7
29	CC	235	GLY	2.7
31	CA	1653	G	2.7
31	CA	2107	G	2.7
31	CA	2125	G	2.7
54	DA	1062	G	2.7
54	DA	2124	G	2.7
11	BK	13	ARG	2.7
16	BP	25	ARG	2.7
19	AS	37	ARG	2.7
9	AI	64	TYR	2.7
9	BI	114	LYS	2.7
23	C2	53	LYS	2.7
40	CN	118	LYS	2.7
50	CX	75	LYS	2.7
32	CE	182	ALA	2.7
48	CV	64	ALA	2.7
13	AM	43	VAL	2.7
37	CK	48	VAL	2.7
41	CO	18	GLN	2.7
44	CR	37	GLN	2.7
13	BM	10	PRO	2.7
20	BT	86	LEU	2.7
23	C2	36	LEU	2.7
31	CA	1396	U	2.7
48	CV	65	ILE	2.7
1	BA	1363	A	2.7
31	CA	1808	A	2.7
54	DA	2142	A	2.7
10	BJ	48	ARG	2.7
14	BN	61	ARG	2.7
50	CX	41	ARG	2.7
9	AI	13	LYS	2.7
41	CO	5	LYS	2.7
47	CU	64	LYS	2.7
47	CU	81	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	CV	79	LYS	2.7
1	AA	995	C	2.7
1	BA	207	C	2.7
1	BA	1322	C	2.7
54	DA	143	C	2.7
13	AM	86	TYR	2.7
7	AG	105	VAL	2.7
1	BA	220	G	2.7
1	BA	1220	G	2.7
1	BA	1221	G	2.7
44	CR	52	GLN	2.7
10	BJ	6	ILE	2.7
16	BP	10	GLY	2.7
30	CD	168	GLU	2.7
39	CM	114	GLY	2.7
16	BP	12	LYS	2.7
1	AA	950	U	2.7
31	CA	654	A	2.7
31	CA	878	A	2.7
31	CA	2872	A	2.7
54	DA	2134	A	2.7
13	AM	5	ALA	2.7
13	AM	106	ALA	2.7
30	CD	65	ALA	2.7
35	DH	25	TYR	2.7
44	CR	21	ALA	2.7
6	AF	61	LEU	2.7
23	C2	11	LEU	2.7
36	DJ	28	LEU	2.7
42	CP	48	LEU	2.7
48	CV	70	VAL	2.7
1	BA	136	C	2.7
1	BA	932	C	2.7
26	C5	31	PRO	2.7
31	CA	128	C	2.7
13	BM	22	ILE	2.7
33	CF	154	ILE	2.7
36	DJ	35	ILE	2.7
36	DJ	67	PHE	2.7
52	CZ	30	MET	2.7
47	CU	12	ARG	2.7
11	BK	68	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	AM	99	GLY	2.7
22	C1	7	LYS	2.7
35	DH	87	GLU	2.7
10	BJ	50	THR	2.7
1	BA	200	G	2.7
1	BA	213	G	2.7
1	BA	954	G	2.7
1	BA	1355	G	2.7
31	CA	317	G	2.7
31	CA	801	G	2.7
31	CA	2286	G	2.7
23	C2	52	ALA	2.7
1	BA	209	U	2.7
10	BJ	77	VAL	2.7
29	CC	228	VAL	2.7
30	CD	122	VAL	2.7
39	CM	58	TYR	2.7
54	DA	546	U	2.7
1	AA	1236	A	2.6
7	BG	42	ILE	2.6
14	AN	31	ILE	2.6
31	CA	504	A	2.6
31	CA	1322	A	2.6
31	CA	1469	A	2.6
31	CA	1525	A	2.6
39	CM	73	ILE	2.6
41	CO	113	ILE	2.6
25	C4	23	LYS	2.6
13	BM	99	GLY	2.6
1	BA	962	C	2.6
9	BI	112	GLU	2.6
10	AJ	38	GLY	2.6
39	CM	28	GLY	2.6
9	AI	35	LEU	2.6
32	CE	52	VAL	2.6
36	DJ	78	VAL	2.6
44	CR	29	SER	2.6
1	BA	976	G	2.6
3	BC	162	ILE	2.6
14	BN	82	ILE	2.6
23	C2	48	ILE	2.6
23	D2	54	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AB	9	MET	2.6
24	C3	41	ARG	2.6
1	BA	1183	U	2.6
15	BO	62	GLN	2.6
31	CA	224	U	2.6
31	CA	790	U	2.6
31	CA	1468	U	2.6
35	CH	11	ASN	2.6
43	CQ	94	LYS	2.6
45	CS	6	GLN	2.6
45	CS	71	LYS	2.6
46	CT	79	GLY	2.6
1	BA	65	A	2.6
37	CK	9	GLU	2.6
54	DA	2119	A	2.6
14	AN	11	VAL	2.6
32	CE	28	VAL	2.6
40	CN	36	VAL	2.6
41	CO	10	LEU	2.6
46	CT	19	LEU	2.6
53	DI	25	ALA	2.6
1	AA	1120	C	2.6
1	BA	1320	C	2.6
31	CA	1985	C	2.6
31	CA	2045	C	2.6
17	BQ	21	ILE	2.6
2	AB	136	MET	2.6
20	BT	33	LYS	2.6
29	CC	255	LYS	2.6
47	CU	30	ILE	2.6
2	AB	201	PRO	2.6
29	CC	8	PRO	2.6
36	DJ	20	PRO	2.6
2	AB	42	ASN	2.6
39	CM	34	GLY	2.6
31	CA	1466	U	2.6
54	DA	102	U	2.6
54	DA	1094	U	2.6
31	CA	107	G	2.6
31	CA	1107	G	2.6
31	CA	1311	G	2.6
31	CA	2110	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	BJ	87	LEU	2.6
7	BG	150	ALA	2.6
19	BS	79	THR	2.6
22	C1	28	LEU	2.6
36	CJ	58	VAL	2.6
41	CO	36	THR	2.6
47	CU	60	THR	2.6
48	CV	2	ALA	2.6
24	C3	28	ARG	2.6
31	CA	676	A	2.6
39	CM	69	ARG	2.6
37	CK	142	ILE	2.6
48	CV	58	ILE	2.6
49	CW	14	LYS	2.6
14	AN	5	SER	2.6
6	AF	88	MET	2.6
48	CV	45	HIS	2.6
7	BG	93	PRO	2.6
1	BA	328	C	2.6
31	CA	444	C	2.6
36	DJ	131	GLY	2.6
51	CY	17	ASN	2.6
23	C2	51	GLU	2.6
39	CM	82	LEU	2.6
39	CM	92	LEU	2.6
48	CV	14	LEU	2.6
2	BB	210	VAL	2.6
7	BG	134	ALA	2.6
9	BI	48	VAL	2.6
29	CC	220	VAL	2.6
32	CE	83	VAL	2.6
49	CW	22	ALA	2.6
52	CZ	53	VAL	2.6
6	BF	91	ARG	2.6
10	BJ	45	ARG	2.6
10	BJ	46	LYS	2.6
30	CD	208	LYS	2.6
31	CA	235	U	2.6
31	CA	355	U	2.6
37	CK	39	LYS	2.6
39	CM	78	ARG	2.6
45	CS	76	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	DA	846[A]	U	2.6
20	BT	83	ILE	2.6
36	DJ	109	ILE	2.6
14	BN	6	MET	2.6
1	BA	102	G	2.6
6	BF	8	PHE	2.6
14	AN	80	SER	2.6
31	CA	312	G	2.6
31	CA	1087	G	2.6
39	CM	64	PHE	2.6
42	CP	32	PRO	2.6
14	BN	4	GLN	2.6
29	DC	251	GLN	2.6
31	CA	354	A	2.6
31	CA	1307	A	2.6
12	BL	109	ASP	2.6
25	C4	53	GLY	2.6
34	DG	114	ASP	2.6
42	CP	93	ASP	2.6
41	CO	98	LEU	2.6
9	AI	17	ALA	2.6
10	BJ	84	VAL	2.6
13	AM	97	VAL	2.6
23	C2	47	VAL	2.6
31	CA	968	C	2.6
35	CH	108	VAL	2.6
36	DJ	57	VAL	2.6
45	CS	48	LYS	2.6
48	CV	15	THR	2.6
36	DJ	59	ILE	2.5
42	CP	87	ILE	2.5
3	BC	37	PHE	2.5
1	BA	981	U	2.5
1	BA	1307	U	2.5
19	BS	14	HIS	2.5
29	CC	6	CYS	2.5
31	CA	276	U	2.5
31	CA	2585	U	2.5
42	CP	29	HIS	2.5
42	CP	5	SER	2.5
36	CJ	53	LEU	2.5
39	CM	27	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	1356	G	2.5
2	BB	82	ASP	2.5
14	BN	53	ARG	2.5
24	C3	9	VAL	2.5
30	CD	26	VAL	2.5
31	CA	117	G	2.5
41	CO	47	VAL	2.5
47	CU	57	VAL	2.5
29	CC	210	ALA	2.5
31	CA	1213	A	2.5
31	CA	1572	A	2.5
31	CA	2587	A	2.5
31	CA	2873	A	2.5
3	BC	44	THR	2.5
36	CJ	73	THR	2.5
25	C4	22	PHE	2.5
3	BC	193	TYR	2.5
19	BS	4	SER	2.5
47	CU	78	SER	2.5
29	CC	217	ARG	2.5
30	CD	62	LYS	2.5
46	CT	98	LYS	2.5
48	CV	47	LYS	2.5
47	CU	67	VAL	2.5
14	AN	25	ALA	2.5
20	BT	70	ASN	2.5
48	CV	40	ASN	2.5
48	CV	103	ILE	2.5
1	BA	205	A	2.5
31	CA	2154	A	2.5
1	BA	1343	G	2.5
31	CA	2405	G	2.5
54	DA	1071	G	2.5
16	AP	41	PRO	2.5
25	C4	64	TYR	2.5
16	BP	52	LEU	2.5
1	BA	1369	C	2.5
12	BL	14	ARG	2.5
32	CE	147	LEU	2.5
47	CU	32	LEU	2.5
30	CD	6	GLY	2.5
31	CA	33	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	BG	32	VAL	2.5
17	BQ	29	VAL	2.5
22	C1	54	VAL	2.5
47	CU	10	VAL	2.5
53	DI	55	VAL	2.5
44	CR	35	ALA	2.5
1	BA	471	U	2.5
31	CA	2713	U	2.5
31	CA	2871	U	2.5
34	CG	103	ILE	2.5
42	DP	1	MET	2.5
2	BB	126	PHE	2.5
9	BI	64	TYR	2.5
20	AT	20	HIS	2.5
25	C4	5	LYS	2.5
1	BA	532	A	2.5
20	BT	65	GLY	2.5
31	CA	1134	A	2.5
50	CX	27	GLY	2.5
10	BJ	64	GLN	2.5
46	CT	29	VAL	2.5
13	BM	85	CYS	2.5
31	CA	619	G	2.5
32	CE	50	ALA	2.5
39	CM	71	ALA	2.5
8	AH	3	MET	2.5
31	CA	11	C	2.5
31	CA	336	C	2.5
31	CA	343	C	2.5
31	CA	623	C	2.5
31	CA	2667	C	2.5
31	CA	2676	C	2.5
31	CA	615	U	2.5
54	DA	2111	U	2.5
22	C1	16	ARG	2.5
24	C3	25	LYS	2.5
32	CE	47	LYS	2.5
32	CE	69	ARG	2.5
33	CF	117	LEU	2.5
3	BC	197	GLY	2.5
29	CC	209	GLY	2.5
32	CE	64	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	CE	81	GLY	2.5
12	BL	4	VAL	2.5
46	CT	71	VAL	2.5
12	AL	2	ALA	2.4
30	DD	54	ALA	2.4
32	CE	39	ALA	2.4
43	CQ	108	ALA	2.4
31	CA	1237	A	2.4
46	CT	86	MET	2.4
7	BG	151	PHE	2.4
27	C0	53	PHE	2.4
3	BC	179	ARG	2.4
12	AL	15	LYS	2.4
14	BN	59	ARG	2.4
48	CV	21	LYS	2.4
30	CD	121	THR	2.4
1	AA	1147	C	2.4
1	BA	210	C	2.4
1	BA	953	G	2.4
10	AJ	73	LEU	2.4
31	CA	46	G	2.4
31	CA	488	G	2.4
31	CA	512	G	2.4
31	CA	729	G	2.4
31	CA	1092	C	2.4
31	CA	1382	G	2.4
31	CA	2066	C	2.4
31	CA	2128	G	2.4
31	CA	2526	G	2.4
32	CE	159	LEU	2.4
51	CY	25	THR	2.4
31	CA	184	C	2.4
52	CZ	21	LEU	2.4
24	C3	7	PRO	2.4
29	CC	247	PRO	2.4
13	AM	23	TYR	2.4
31	CA	1066	U	2.4
24	C3	27	GLY	2.4
39	CM	20	GLY	2.4
41	CO	7	GLY	2.4
11	BK	67	ALA	2.4
24	C3	20	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	BQ	63	GLU	2.4
7	BG	36	LYS	2.4
50	CX	60	PHE	2.4
27	C0	17	LEU	2.4
1	BA	101	A	2.4
14	BN	54	ASP	2.4
22	C1	26	THR	2.4
3	BC	2	GLY	2.4
32	CE	96	VAL	2.4
45	CS	12	HIS	2.4
1	AA	1141	C	2.4
1	BA	984	C	2.4
12	BL	17	ALA	2.4
19	AS	50	ALA	2.4
31	CA	876	C	2.4
31	CA	1161	C	2.4
31	CA	1607	C	2.4
31	CA	2527	C	2.4
31	CA	2691	C	2.4
36	DJ	63	ALA	2.4
45	CS	36	ALA	2.4
1	AA	632	U	2.4
1	AA	1126	U	2.4
1	BA	933	G	2.4
1	BA	1286	U	2.4
11	BK	64	GLN	2.4
31	CA	185	G	2.4
31	CA	333	G	2.4
31	CA	583	G	2.4
31	CA	1622	G	2.4
31	CA	1880	U	2.4
31	CA	1971	U	2.4
31	CA	2061	G	2.4
48	CV	46	GLN	2.4
25	C4	12	LYS	2.4
36	CJ	69	PHE	2.4
48	CV	6	ARG	2.4
32	CE	80	SER	2.4
41	CO	79	LEU	2.4
13	AM	104	THR	2.4
33	CF	157	THR	2.4
39	CM	56	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	BJ	60	ASP	2.4
42	CP	103	VAL	2.4
32	CE	42	GLY	2.4
48	CV	38	GLY	2.4
1	AA	199	A	2.4
1	AA	1130	A	2.4
1	BA	977	A	2.4
1	BA	1251	A	2.4
31	CA	457	A	2.4
31	CA	2741	A	2.4
36	CJ	101	ILE	2.4
54	DA	1073	A	2.4
19	AS	7	LYS	2.4
47	DU	69	ARG	2.4
9	BI	20	PHE	2.4
16	BP	32	PHE	2.4
1	BA	458	U	2.4
8	AH	91	GLU	2.4
31	CA	61	C	2.4
31	CA	288	U	2.4
31	CA	2628	C	2.4
34	CG	33	LEU	2.4
54	DA	1060	U	2.4
7	AG	41	SER	2.4
41	CO	15	SER	2.4
1	AA	844	G	2.4
1	BA	326	G	2.4
1	BA	1064	G	2.4
1	BA	1260	G	2.4
31	CA	252	G	2.4
31	CA	1236	G	2.4
31	CA	1444	G	2.4
31	CA	1573	G	2.4
31	CA	2630	G	2.4
36	CJ	126	THR	2.4
45	CS	51	VAL	2.4
48	CV	25	VAL	2.4
22	C1	42	HIS	2.4
3	BC	168	TYR	2.4
16	BP	4	ILE	2.4
29	CC	5	LYS	2.4
36	CJ	10	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	CV	43	LYS	2.4
20	AT	28	MET	2.4
32	CE	46	GLN	2.4
40	CN	22	GLN	2.4
33	DF	117	LEU	2.4
1	AA	964	A	2.4
1	AA	1289	A	2.4
31	CA	614	A	2.4
31	CA	764	A	2.4
31	CA	877	A	2.4
31	CA	2287	A	2.4
43	CQ	102	GLU	2.4
54	DA	2176	A	2.4
30	CD	9	VAL	2.4
31	CA	2891	U	2.4
36	CJ	75	PRO	2.4
48	CV	55	PRO	2.4
1	AA	210	C	2.3
1	BA	985	C	2.3
31	CA	517	C	2.3
31	CA	1319	C	2.3
31	CA	1708	C	2.3
31	CA	2065	C	2.3
9	AI	72	ILE	2.3
9	BI	31	ASN	2.3
9	BI	108	ALA	2.3
9	BI	129	LYS	2.3
19	AS	11	ILE	2.3
22	C1	6	ASN	2.3
27	C0	20	HIS	2.3
29	CC	18	LYS	2.3
38	CL	16	ALA	2.3
41	CO	45	ARG	2.3
47	DU	2	ILE	2.3
48	CV	27	ASN	2.3
53	DI	91	ALA	2.3
16	BP	23	ASP	2.3
1	AA	540	G	2.3
1	BA	942	G	2.3
1	BA	1222	G	2.3
31	CA	1252	G	2.3
2	BB	162	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	16	LEU	2.3
42	CP	97	PHE	2.3
7	AG	94	VAL	2.3
9	AI	48	VAL	2.3
46	CT	47	VAL	2.3
53	DI	26	VAL	2.3
7	AG	2	PRO	2.3
5	BE	103	THR	2.3
7	BG	76	LYS	2.3
10	BJ	67	ILE	2.3
19	AS	77	THR	2.3
19	BS	7	LYS	2.3
22	C1	37	LYS	2.3
31	CA	73	A	2.3
31	CA	222	A	2.3
31	CA	472	A	2.3
25	C4	17	THR	2.3
39	CM	13	LYS	2.3
40	CN	40	ARG	2.3
48	CV	78	GLY	2.3
12	BL	2	ALA	2.3
14	BN	2	ALA	2.3
29	CC	54	ILE	2.3
36	CJ	114	ALA	2.3
39	CM	83	ALA	2.3
53	DI	112	ALA	2.3
20	BT	3	ASN	2.3
31	CA	234	U	2.3
1	BA	1066	C	2.3
31	CA	455	C	2.3
44	CR	18	LEU	2.3
1	BA	203	G	2.3
31	CA	409	G	2.3
31	CA	1309	G	2.3
33	CF	25	VAL	2.3
54	DA	1074	G	2.3
54	DA	2121	G	2.3
13	BM	103	LYS	2.3
27	C0	6	LYS	2.3
25	C4	42	ARG	2.3
41	CO	2	ARG	2.3
47	CU	76	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AC	103	ILE	2.3
36	DJ	25	GLY	2.3
32	CE	131	THR	2.3
39	CM	68	SER	2.3
51	CY	34	HIS	2.3
29	CC	37	ASN	2.3
46	CT	40	ASN	2.3
53	DI	41	LEU	2.3
1	BA	109	A	2.3
19	BS	74	PHE	2.3
32	CE	168	ASP	2.3
42	CP	2	ASP	2.3
1	BA	1065	U	2.3
31	CA	1390	U	2.3
31	CA	2408	U	2.3
54	DA	138	U	2.3
21	BU	44	GLU	2.3
34	CG	32	GLU	2.3
31	CA	426	C	2.3
54	DA	1072	C	2.3
9	AI	11	ARG	2.3
15	AO	72	ARG	2.3
20	BT	10	ARG	2.3
44	CR	6	ARG	2.3
3	AC	74	GLY	2.3
10	AJ	100	ILE	2.3
41	CO	109	PRO	2.3
38	CL	68	GLY	2.3
25	C4	48	ALA	2.3
2	AB	46	THR	2.3
7	AG	116	MET	2.3
30	CD	133	THR	2.3
41	CO	20	MET	2.3
14	AN	16	LEU	2.3
21	AU	16	LEU	2.3
24	C3	16	HIS	2.3
48	CV	98	SER	2.3
29	CC	33	LEU	2.3
9	AI	39	PHE	2.3
9	BI	39	PHE	2.3
31	CA	289	G	2.3
31	CA	408	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	1514	G	2.3
31	CA	2802	G	2.3
48	CV	87	PHE	2.3
3	BC	118	ASP	2.3
13	BM	100	GLN	2.3
47	CU	79	ASP	2.3
50	CX	15	ASP	2.3
29	CC	28	LYS	2.3
30	CD	157	LYS	2.3
46	CT	6	LYS	2.3
7	BG	109	ARG	2.3
13	AM	64	VAL	2.3
22	C1	40	ARG	2.3
31	CA	227	A	2.3
1	BA	218	U	2.3
31	CA	448	U	2.3
31	CA	810	U	2.3
54	DA	2106	U	2.3
13	AM	4	ILE	2.3
14	BN	52	PRO	2.3
51	CY	59	ILE	2.3
5	BE	127	ALA	2.3
24	C3	32	ALA	2.3
39	CM	52	GLY	2.3
14	AN	42	TRP	2.3
31	CA	237	C	2.3
31	CA	456	C	2.3
31	CA	1005	C	2.3
31	CA	2150	C	2.3
31	CA	2248	C	2.3
31	CA	2338	C	2.3
31	CA	2443	C	2.3
7	BG	13	LEU	2.3
7	BG	124	LEU	2.3
36	CJ	138	LEU	2.3
47	CU	7	LEU	2.3
52	CZ	43	LEU	2.3
19	AS	69	HIS	2.3
7	BG	41	SER	2.3
14	BN	32	SER	2.3
9	BI	13	LYS	2.3
9	BI	123	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	AM	100	GLN	2.3
19	BS	17	LYS	2.3
32	CE	57	LYS	2.3
34	CG	176	LYS	2.3
24	C3	33	ARG	2.3
25	C4	13	ARG	2.3
29	CC	14	ARG	2.3
16	BP	53	ASP	2.3
25	C4	50	VAL	2.3
48	CV	37	GLU	2.2
31	CA	7	G	2.2
31	CA	1524	G	2.2
31	CA	2190	G	2.2
54	DA	141	G	2.2
3	AC	162	ILE	2.2
44	CR	99	ALA	2.2
1	AA	960	U	2.2
1	BA	114	U	2.2
1	BA	199	A	2.2
1	BA	1288	A	2.2
7	AG	50	LEU	2.2
7	AG	59	LEU	2.2
31	CA	686	U	2.2
31	CA	1406	U	2.2
39	CM	3	LEU	2.2
46	CT	36	LEU	2.2
54	DA	12	U	2.2
54	DA	1420	A	2.2
54	DA	2155	U	2.2
19	AS	79	THR	2.2
25	C4	51	SER	2.2
29	DC	38	SER	2.2
33	CF	128	TYR	2.2
36	CJ	128	SER	2.2
1	BA	135	C	2.2
24	C3	19	ARG	2.2
28	CB	30	C	2.2
31	CA	2078	C	2.2
31	CA	2362	C	2.2
48	CV	22	ARG	2.2
54	DA	1100	C	2.2
2	BB	70	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	CE	196	VAL	2.2
40	CN	17	ASN	2.2
49	CW	89	ILE	2.2
53	DI	123	ILE	2.2
14	AN	52	PRO	2.2
8	BH	121	LEU	2.2
16	BP	82	ALA	2.2
27	C0	29	LEU	2.2
43	CQ	91	ALA	2.2
47	CU	83	ALA	2.2
1	AA	1290	G	2.2
1	BA	260	G	2.2
7	AG	25	LYS	2.2
13	BM	110	LYS	2.2
36	DJ	42	PHE	2.2
18	BR	74	HIS	2.2
19	BS	39	THR	2.2
31	CA	124	G	2.2
31	CA	214	G	2.2
31	CA	1093	G	2.2
31	CA	2742	G	2.2
9	BI	130	ARG	2.2
29	CC	48	ARG	2.2
31	CA	102	U	2.2
39	CM	47	ARG	2.2
53	DI	84	TYR	2.2
54	DA	2130	U	2.2
1	BA	1280	A	2.2
14	BN	56	SER	2.2
31	CA	483	A	2.2
31	CA	626	A	2.2
31	CA	2059	A	2.2
31	CA	2820	A	2.2
36	DJ	128	SER	2.2
46	CT	13	SER	2.2
10	BJ	57	VAL	2.2
30	CD	60	VAL	2.2
35	CH	144	VAL	2.2
36	CJ	139	VAL	2.2
36	DJ	70	VAL	2.2
1	AA	470	C	2.2
1	AA	1066	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	31	C	2.2
31	CA	236	C	2.2
31	CA	672	C	2.2
31	CA	2347	C	2.2
7	BG	59	LEU	2.2
17	BQ	44	LEU	2.2
41	CO	106	ASP	2.2
48	CV	18	ASP	2.2
51	CY	24	ALA	2.2
32	CE	23	PHE	2.2
29	CC	271	ARG	2.2
17	BQ	42	THR	2.2
37	CK	40	HIS	2.2
46	CT	7	HIS	2.2
10	AJ	36	VAL	2.2
44	CR	31	VAL	2.2
1	AA	1354	U	2.2
1	BA	1121	U	2.2
28	CB	74	U	2.2
31	CA	2384	U	2.2
54	DA	139	U	2.2
54	DA	360	U	2.2
54	DA	1081	U	2.2
7	BG	104	ILE	2.2
48	CV	72	ILE	2.2
1	AA	76	G	2.2
13	BM	105	ASN	2.2
1	BA	468	A	2.2
4	AD	21	LEU	2.2
29	CC	35	GLU	2.2
31	CA	182	A	2.2
31	CA	250	G	2.2
31	CA	338	G	2.2
31	CA	432	A	2.2
31	CA	735	A	2.2
31	CA	777	G	2.2
31	CA	989	G	2.2
31	CA	1300	G	2.2
31	CA	2112	G	2.2
54	DA	2112	G	2.2
52	CZ	19	LEU	2.2
52	CZ	22	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	DI	3	LEU	2.2
7	BG	71	PRO	2.2
32	CE	34	ALA	2.2
39	CM	102	GLY	2.2
10	AJ	91	ASP	2.2
12	BL	15	LYS	2.2
30	CD	116	LYS	2.2
44	CR	78	LYS	2.2
53	DI	37	LYS	2.2
14	BN	21	PHE	2.2
19	AS	10	PHE	2.2
30	CD	59	ARG	2.2
39	CM	107	PHE	2.2
31	CA	264	C	2.2
31	CA	510	C	2.2
9	BI	9	THR	2.2
36	CJ	57	VAL	2.2
9	AI	110	GLN	2.2
14	BN	80	SER	2.2
32	CE	94	GLN	2.2
14	BN	51	LEU	2.2
18	BR	67	LEU	2.2
52	CZ	42	LEU	2.2
5	BE	110	ALA	2.2
11	AK	66	ALA	2.2
19	AS	75	ALA	2.2
36	CJ	83	ALA	2.2
36	DJ	110	ALA	2.2
42	CP	20	GLU	2.2
1	AA	1125	U	2.2
2	BB	98	GLY	2.2
13	AM	26	GLY	2.2
13	AM	31	LYS	2.2
40	CN	58	LYS	2.2
45	CS	28	ALA	2.2
46	CT	64	ALA	2.2
31	CA	2743	U	2.2
33	CF	84	PRO	2.2
10	BJ	9	ARG	2.2
50	CX	25	ARG	2.2
10	BJ	91	ASP	2.2
16	BP	39	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	CE	183	PHE	2.2
45	CS	77	PHE	2.2
47	CU	37	ASP	2.2
52	DZ	49	ASP	2.2
1	AA	978	A	2.2
1	AA	1285	A	2.2
54	DA	1098	A	2.2
54	DA	2135	A	2.2
54	DA	2170	A	2.2
1	BA	1124	G	2.2
31	CA	277	G	2.2
31	CA	308	G	2.2
31	CA	974	G	2.2
31	CA	1099	G	2.2
31	CA	1341	G	2.2
7	BG	135	VAL	2.1
32	CE	65	THR	2.1
36	DJ	68	THR	2.1
45	CS	96	VAL	2.1
1	AA	1129	C	2.1
2	BB	164	ILE	2.1
5	AE	164	ILE	2.1
13	BM	7	ILE	2.1
31	CA	151	C	2.1
31	CA	791	C	2.1
31	CA	1526	C	2.1
3	BC	12	LEU	2.1
7	AG	30	LEU	2.1
7	BG	50	LEU	2.1
9	BI	63	LEU	2.1
10	BJ	90	LEU	2.1
14	BN	49	GLN	2.1
14	BN	66	GLN	2.1
23	C2	33	LYS	2.1
14	AN	29	ALA	2.1
15	BO	2	SER	2.1
36	DJ	14	ALA	2.1
44	CR	27	ALA	2.1
52	CZ	63	ALA	2.1
9	AI	18	ARG	2.1
29	CC	227	PRO	2.1
29	CC	238	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	CJ	89	GLY	2.1
36	DJ	137	GLY	2.1
38	CL	120	PRO	2.1
42	CP	16	ARG	2.1
21	BU	12	PHE	2.1
32	CE	158	PHE	2.1
45	CS	35	PHE	2.1
1	AA	1307	U	2.1
13	AM	11	ASP	2.1
26	C5	20	ASP	2.1
31	CA	34	U	2.1
31	CA	392	U	2.1
31	CA	431	U	2.1
31	CA	1647	U	2.1
54	DA	1083	U	2.1
54	DA	1105	U	2.1
54	DA	2139	U	2.1
6	AF	42	TRP	2.1
35	CH	130	VAL	2.1
1	BA	1016	A	2.1
7	AG	12	ILE	2.1
13	BM	23	TYR	2.1
20	BT	57	ILE	2.1
31	CA	226	A	2.1
31	CA	616	A	2.1
31	CA	1143	A	2.1
31	CA	1395	A	2.1
37	CK	103	ILE	2.1
54	DA	1086	A	2.1
3	BC	33	LEU	2.1
6	BF	93	LYS	2.1
12	BL	108	LYS	2.1
30	CD	201	LEU	2.1
40	CN	41	LEU	2.1
10	BJ	68	ARG	2.1
31	CA	98	G	2.1
31	CA	356	G	2.1
31	CA	530	G	2.1
31	CA	1239	G	2.1
31	CA	1388	G	2.1
31	CA	1407	G	2.1
31	CA	1627	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	2136	G	2.1
38	CL	1	MET	2.1
36	CJ	133	ALA	2.1
37	CK	116	ARG	2.1
45	CS	84	ARG	2.1
46	DT	110	ARG	2.1
54	DA	548	G	2.1
29	CC	112	ALA	2.1
49	CW	23	ALA	2.1
23	C2	4	GLY	2.1
32	CE	55	SER	2.1
36	CJ	130	GLU	2.1
1	AA	932	C	2.1
1	AA	1119	C	2.1
1	BA	611	C	2.1
31	CA	357	C	2.1
31	CA	1934	C	2.1
16	BP	26	ASN	2.1
35	DH	20	ASN	2.1
7	AG	33	ASP	2.1
19	AS	67	VAL	2.1
29	CC	229	ASP	2.1
32	CE	187	VAL	2.1
48	CV	34	VAL	2.1
1	AA	208	U	2.1
8	BH	32	LEU	2.1
12	BL	44	LYS	2.1
13	AM	27	LYS	2.1
19	AS	33	THR	2.1
25	C4	62	LEU	2.1
29	CC	223	THR	2.1
30	CD	25	THR	2.1
29	CC	62	TYR	2.1
31	CA	72	U	2.1
31	CA	290	U	2.1
31	CA	766	U	2.1
31	CA	2506	U	2.1
32	CE	84	THR	2.1
36	CJ	132	THR	2.1
47	CU	2	ILE	2.1
48	CV	41	LEU	2.1
5	BE	93	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	AR	73	ARG	2.1
24	C3	21	ARG	2.1
52	CZ	48	ARG	2.1
2	BB	89	GLN	2.1
44	CR	44	GLN	2.1
51	CY	53	ALA	2.1
1	BA	1146	A	2.1
2	BB	149	GLY	2.1
31	CA	443	A	2.1
31	CA	631	A	2.1
43	CQ	22	PRO	2.1
44	CR	73	GLY	2.1
54	DA	1088	A	2.1
7	AG	151	PHE	2.1
14	AN	100	SER	2.1
29	CC	240	PHE	2.1
45	CS	53	PHE	2.1
1	AA	212	G	2.1
1	BA	134	G	2.1
1	BA	606	G	2.1
1	BA	1353	G	2.1
11	AK	129	VAL	2.1
31	CA	1168	G	2.1
31	CA	1346	G	2.1
31	CA	1455	G	2.1
36	CJ	61	VAL	2.1
51	CY	4	VAL	2.1
54	DA	1059	G	2.1
1	BA	214	C	2.1
1	BA	1237	C	2.1
1	BA	1245	C	2.1
31	CA	736	C	2.1
31	CA	1730	C	2.1
54	DA	2178	C	2.1
14	BN	98	LYS	2.1
29	CC	265	LYS	2.1
32	CE	60	TRP	2.1
39	CM	36	LYS	2.1
44	CR	16	LYS	2.1
51	CY	26	LYS	2.1
11	AK	97	ILE	2.1
14	BN	63	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	CU	77	ARG	2.1
22	C1	49	TYR	2.1
16	BP	81	ALA	2.1
1	BA	843	U	2.1
1	BA	1123	U	2.1
31	CA	1234	U	2.1
31	CA	1467	U	2.1
31	CA	1709	U	2.1
31	CA	2244	U	2.1
54	DA	1058	U	2.1
29	CC	249	GLY	2.1
2	BB	201	PRO	2.1
4	AD	88	GLU	2.1
26	C5	30	GLU	2.1
34	CG	83	PHE	2.1
43	CQ	34	GLU	2.1
48	CV	50	PRO	2.1
51	CY	46	PHE	2.1
47	CU	31	VAL	2.1
53	DI	77	VAL	2.1
1	BA	1285	A	2.1
7	AG	110	LYS	2.1
31	CA	219	A	2.1
31	CA	1597	A	2.1
32	CE	97	ASN	2.1
53	DI	103	ASN	2.1
2	BB	57	LEU	2.1
2	BB	148	LEU	2.1
10	BJ	62	ARG	2.1
37	CK	93	ILE	2.1
39	CM	105	ILE	2.1
12	BL	117	TYR	2.1
23	C2	17	THR	2.1
26	C5	1	MET	2.1
27	C0	8	THR	2.1
32	CE	43	THR	2.1
32	CE	173	THR	2.1
34	CG	157	TYR	2.1
1	AA	1245	C	2.1
1	AA	1302	C	2.1
1	BA	1281	C	2.1
1	BA	1352	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	1533	C	2.1
14	AN	8	ALA	2.1
28	CB	97	C	2.1
31	CA	1461	C	2.1
53	DI	92	ALA	2.1
54	DA	2160	C	2.1
31	CA	51	G	2.1
31	CA	180	G	2.1
31	CA	245	G	2.1
31	CA	618	G	2.1
31	CA	1248	G	2.1
31	CA	1380	G	2.1
31	CA	1767	G	2.1
31	CA	1807	G	2.1
31	CA	1878	G	2.1
31	CA	2120	G	2.1
31	CA	2148	G	2.1
31	CA	2152	G	2.1
54	DA	1171	G	2.1
30	CD	144	GLY	2.1
46	CT	31	GLN	2.1
47	CU	65	GLY	2.1
49	CW	87	GLN	2.1
10	BJ	55	PRO	2.1
24	C3	18	PHE	2.1
32	CE	59	PRO	2.1
35	CH	132	PHE	2.1
2	BB	92	VAL	2.0
7	BG	64	VAL	2.0
7	BG	80	VAL	2.0
9	AI	111	VAL	2.0
14	BN	3	LYS	2.0
30	CD	207	VAL	2.0
31	CA	459	U	2.0
31	CA	1209	U	2.0
31	CA	1397	U	2.0
31	CA	2079	U	2.0
31	CA	2249	U	2.0
20	AT	6	SER	2.0
23	C2	14	SER	2.0
41	CO	6	SER	2.0
53	DI	30	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	BK	97	ILE	2.0
13	AM	98	ARG	2.0
39	CM	18	ARG	2.0
41	CO	107	ASN	2.0
1	AA	1332	A	2.0
9	BI	43	THR	2.0
12	BL	64	THR	2.0
12	BL	113	ALA	2.0
14	AN	20	TYR	2.0
22	C1	20	ASP	2.0
24	C3	36	ALA	2.0
31	CA	1387	A	2.0
31	CA	1566	A	2.0
36	CJ	63	ALA	2.0
54	DA	2126	A	2.0
54	DA	2171	A	2.0
7	AG	34	GLY	2.0
19	AS	68	GLY	2.0
44	CR	71	GLN	2.0
1	AA	207	C	2.0
6	AF	93	LYS	2.0
9	BI	115	LYS	2.0
20	AT	16	LYS	2.0
44	CR	19	LYS	2.0
45	CS	37	GLU	2.0
31	CA	337	C	2.0
31	CA	581	C	2.0
31	CA	1345	C	2.0
31	CA	2073	C	2.0
46	CT	42	LYS	2.0
24	C3	30	VAL	2.0
36	DJ	140	VAL	2.0
51	CY	47	VAL	2.0
7	BG	23	LEU	2.0
15	AO	17	ARG	2.0
22	C1	39	LEU	2.0
25	C4	8	ARG	2.0
31	CA	1	G	2.0
31	CA	388	G	2.0
31	CA	690	G	2.0
31	CA	1862	G	2.0
31	CA	2693	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	AS	4	SER	2.0
27	C0	7	ILE	2.0
27	C0	48	ILE	2.0
41	CO	34	ILE	2.0
1	BA	252	U	2.0
25	C4	49	MET	2.0
47	CU	80	TRP	2.0
6	BF	92	THR	2.0
10	AJ	80	THR	2.0
7	BG	15	ASP	2.0
37	CK	49	ASP	2.0
10	BJ	49	PHE	2.0
23	C2	18	GLY	2.0
51	CY	38	PHE	2.0
4	BD	40	GLN	2.0
9	AI	23	PRO	2.0
12	BL	91	PRO	2.0
32	CE	74	LYS	2.0
33	CF	15	LYS	2.0
36	DJ	26	PRO	2.0
40	CN	72	PRO	2.0
46	CT	80	PRO	2.0
49	CW	27	PRO	2.0
1	AA	1092	A	2.0
1	BA	223	A	2.0
2	AB	210	VAL	2.0
16	BP	20	VAL	2.0
31	CA	477	A	2.0
31	CA	507	A	2.0
31	CA	1596	A	2.0
31	CA	2020	A	2.0
24	C3	12	ARG	2.0
26	C5	12	ARG	2.0
32	CE	61	ARG	2.0
36	CJ	70	VAL	2.0
42	CP	27	VAL	2.0
44	CR	50	ARG	2.0
52	CZ	46	VAL	2.0
2	AB	135	LEU	2.0
13	BM	56	LEU	2.0
14	BN	74	LEU	2.0
33	CF	36	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	BH	36	ILE	2.0
33	CF	67	ILE	2.0
36	DJ	122	ILE	2.0
1	AA	206	C	2.0
1	BA	234	C	2.0
31	CA	32	C	2.0
31	CA	1320	C	2.0
31	CA	1574	C	2.0
31	CA	2678	C	2.0
54	DA	2161	C	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	1207	24/25	0.63	0.12	158,159,162,165	0
1	2MG	BA	966	24/25	0.66	0.15	149,153,160,161	0
1	5MC	BA	967	21/22	0.74	0.15	148,154,156,157	0
31	PSU	CA	1917	20/21	0.76	0.11	118,126,134,134	0
31	2MA	CA	2503	23/24	0.84	0.18	90,96,102,102	0
1	2MG	AA	1207	24/25	0.85	0.12	113,117,120,122	0
31	3TD	CA	1915	21/22	0.85	0.09	146,150,155,155	0
31	PSU	CA	1911	20/21	0.86	0.08	111,128,131,132	0
31	PSU	CA	746	20/21	0.86	0.12	93,99,101,102	0
31	PSU	CA	2504	20/21	0.86	0.16	78,86,90,91	0
31	PSU	CA	2457	20/21	0.87	0.12	79,83,85,85	0
31	6MZ	CA	1618	23/24	0.87	0.13	98,107,108,109	0
31	PSU	CA	955	20/21	0.87	0.12	84,89,90,90	0
31	PSU	CA	2580	20/21	0.87	0.11	77,86,88,89	0
1	PSU	BA	516	20/21	0.88	0.10	91,96,99,102	0
31	6MZ	CA	2030	23/24	0.88	0.14	78,86,97,99	0
12	D2T	BL	89	10/11	0.89	0.16	81,86,96,96	0
54	3TD	DA	1915	21/22	0.89	0.10	86,90,102,103	0
30	MEQ	CD	150	9/11	0.89	0.19	81,87,117,120	0
1	2MG	AA	966	24/25	0.90	0.11	78,87,97,97	0
54	PSU	DA	1917	20/21	0.91	0.09	63,73,79,79	0
31	5MC	CA	1962	21/22	0.91	0.14	67,72,76,76	0
31	5MU	CA	1939	21/22	0.92	0.12	69,74,80,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	1MG	CA	745	24/25	0.92	0.12	85,87,90,93	0
12	D2T	AL	89	10/11	0.92	0.12	47,53,67,70	0
40	4D4	CN	81	12/13	0.92	0.12	83,89,102,103	0
31	G7M	CA	2069	24/25	0.92	0.16	78,83,88,88	0
31	2MG	CA	2445	24/25	0.92	0.17	66,75,80,83	0
31	2MG	CA	1835	24/25	0.92	0.11	60,73,76,78	0
1	UR3	BA	1498	21/22	0.93	0.10	78,80,84,84	0
31	5MU	CA	747	21/22	0.93	0.10	93,100,102,105	0
31	OMC	CA	2498	21/22	0.93	0.12	77,80,86,87	0
1	PSU	AA	516	20/21	0.93	0.08	68,72,78,78	0
1	5MC	BA	1407	21/22	0.93	0.11	81,95,99,100	0
1	G7M	BA	527	24/25	0.94	0.09	80,85,91,93	0
1	5MC	AA	967	21/22	0.94	0.10	76,93,96,97	0
31	OMG	CA	2251	24/25	0.94	0.13	67,73,75,77	0
1	2MG	BA	1516	24/25	0.94	0.09	61,67,78,80	0
31	OMU	CA	2552	21/22	0.94	0.17	78,81,85,89	0
1	MA6	BA	1518	24/25	0.95	0.09	67,74,79,79	0
31	PSU	CA	2605	20/21	0.95	0.09	74,75,78,80	0
31	PSU	CA	2604	20/21	0.95	0.08	65,71,84,84	0
54	PSU	DA	1911	20/21	0.96	0.06	67,74,75,75	0
1	UR3	AA	1498	21/22	0.96	0.08	51,53,57,59	0
1	4OC	BA	1402	22/23	0.96	0.07	74,79,81,82	0
1	G7M	AA	527	24/25	0.96	0.08	53,59,62,65	0
1	MA6	BA	1519	24/25	0.96	0.09	68,73,77,78	0
40	4D4	DN	81[A]	12/13	0.97	0.10	26,33,49,50	9
40	4D4	DN	81[B]	12/13	0.97	0.10	11,21,28,29	9
54	2MG	DA	1835	24/25	0.97	0.07	31,42,47,48	0
1	4OC	AA	1402	22/23	0.97	0.07	48,55,61,62	0
1	2MG	AA	1516	24/25	0.97	0.08	44,49,52,53	0
1	MA6	AA	1518	24/25	0.97	0.08	44,46,50,53	0
54	PSU	DA	2604	20/21	0.97	0.08	32,36,47,47	0
1	MA6	AA	1519	24/25	0.97	0.08	46,48,50,54	0
1	5MC	AA	1407	21/22	0.97	0.06	43,47,52,53	0
54	2MA	DA	2503	23/24	0.98	0.06	15,28,32,41	0
54	PSU	DA	2504	20/21	0.98	0.06	31,33,36,38	0
54	OMU	DA	2552	21/22	0.98	0.07	22,26,30,35	0
54	5MU	DA	747	21/22	0.98	0.06	20,25,31,38	0
54	PSU	DA	2605	20/21	0.98	0.07	26,34,37,38	0
54	5MU	DA	1939	21/22	0.98	0.07	25,30,36,40	0
30	MEQ	DD	150[A]	10/11	0.98	0.07	11,18,25,27	10
30	MEQ	DD	150[B]	10/11	0.98	0.07	19,28,34,35	10
54	5MC	DA	1962	21/22	0.98	0.07	28,37,39,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	DA	2457	20/21	0.99	0.05	22,25,26,29	0
54	OMC	DA	2498	21/22	0.99	0.05	18,21,24,27	0
54	PSU	DA	955	20/21	0.99	0.06	20,23,26,26	0
54	6MZ	DA	1618	23/24	0.99	0.05	17,24,27,28	0
54	PSU	DA	746	20/21	0.99	0.06	18,23,26,30	0
54	PSU	DA	2580	20/21	0.99	0.06	17,21,28,29	0
54	1MG	DA	745	24/25	0.99	0.05	16,22,28,30	0
54	6MZ	DA	2030	23/24	0.99	0.05	15,20,26,28	0
54	G7M	DA	2069	24/25	0.99	0.06	20,28,31,33	0
54	OMG	DA	2251	24/25	0.99	0.05	21,25,34,42	0
54	2MG	DA	2445	24/25	0.99	0.06	16,22,24,25	0
54	H2U	DA	2449	20/21	0.99	0.05	19,22,24,26	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1622	1/1	0.29	0.42	116,116,116,116	0
55	MG	BA	1646	1/1	0.31	0.34	141,141,141,141	0
55	MG	CA	3154	1/1	0.31	0.34	136,136,136,136	0
55	MG	CA	3075	1/1	0.33	0.35	221,221,221,221	0
55	MG	CA	3005	1/1	0.46	0.23	239,239,239,239	0
55	MG	BA	1641	1/1	0.48	0.30	121,121,121,121	0
55	MG	CA	3122	1/1	0.52	0.58	106,106,106,106	0
55	MG	CA	3038	1/1	0.55	0.12	258,258,258,258	0
55	MG	BA	1603	1/1	0.55	0.12	279,279,279,279	0
55	MG	CA	3155	1/1	0.55	0.24	152,152,152,152	0
55	MG	CA	3067	1/1	0.56	0.19	277,277,277,277	0
55	MG	DA	3168	1/1	0.56	0.32	106,106,106,106	0
55	MG	CA	3146	1/1	0.59	0.25	164,164,164,164	0
55	MG	CA	3124	1/1	0.60	0.21	124,124,124,124	0
55	MG	CA	3034	1/1	0.62	0.26	244,244,244,244	0
55	MG	AA	1628	1/1	0.62	0.22	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1607	1/1	0.64	0.27	203,203,203,203	0
55	MG	BA	1638	1/1	0.65	0.52	107,107,107,107	0
55	MG	CA	3135	1/1	0.65	0.50	107,107,107,107	0
55	MG	AA	1677	1/1	0.66	0.15	138,138,138,138	0
55	MG	BA	1606	1/1	0.66	0.25	251,251,251,251	0
55	MG	CA	3077	1/1	0.67	0.21	232,232,232,232	0
55	MG	AA	1678	1/1	0.68	0.28	76,76,76,76	0
55	MG	CA	3060	1/1	0.69	0.17	234,234,234,234	0
55	MG	CA	3061	1/1	0.69	0.11	225,225,225,225	0
55	MG	BA	1624	1/1	0.69	0.13	249,249,249,249	0
55	MG	CA	3148	1/1	0.70	0.44	46,46,46,46	1
55	MG	CA	3139	1/1	0.70	0.20	83,83,83,83	0
55	MG	CA	3132	1/1	0.71	0.24	97,97,97,97	0
55	MG	CA	3110	1/1	0.72	0.23	102,102,102,102	0
55	MG	CA	3002	1/1	0.73	0.15	258,258,258,258	0
55	MG	CA	3104	1/1	0.73	0.21	254,254,254,254	0
55	MG	CA	3123	1/1	0.73	0.14	115,115,115,115	0
57	MPD	DE	301	8/8	0.73	0.25	123,126,129,129	0
59	TAC	BA	1644	32/32	0.73	0.22	139,152,159,159	0
55	MG	DA	3144	1/1	0.74	0.26	107,107,107,107	0
55	MG	CA	3152	1/1	0.74	0.14	145,145,145,145	0
55	MG	CA	3147	1/1	0.74	0.51	51,51,51,51	1
55	MG	BA	1639	1/1	0.74	0.27	93,93,93,93	0
61	PEG	DQ	201	7/7	0.74	0.24	104,108,109,109	0
55	MG	BA	1636	1/1	0.75	0.38	91,91,91,91	0
55	MG	AA	1660	1/1	0.75	0.18	281,281,281,281	0
55	MG	CA	3003	1/1	0.75	0.32	270,270,270,270	0
55	MG	CA	3125	1/1	0.76	0.28	98,98,98,98	0
55	MG	AA	1624	1/1	0.76	0.31	93,93,93,93	0
55	MG	CA	3047	1/1	0.76	0.38	238,238,238,238	0
55	MG	CA	3009	1/1	0.76	0.26	240,240,240,240	0
55	MG	AA	1617	1/1	0.76	0.71	147,147,147,147	0
62	EDO	DA	3003	4/4	0.76	0.29	89,89,89,89	0
66	ACY	DA	3196	4/4	0.76	0.28	72,76,77,77	0
55	MG	CA	3111	1/1	0.77	0.19	76,76,76,76	0
58	PUT	AA	1673	6/6	0.77	0.17	92,93,93,94	0
55	MG	AA	1654	1/1	0.77	0.40	259,259,259,259	0
55	MG	CA	3156	1/1	0.77	0.16	218,218,218,218	0
55	MG	CA	3032	1/1	0.77	0.12	244,244,244,244	0
55	MG	AA	1616	1/1	0.77	0.34	87,87,87,87	0
55	MG	CA	3129	1/1	0.78	0.20	89,89,89,89	0
55	MG	BA	1625	1/1	0.78	0.19	251,251,251,251	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MPD	DK	201	8/8	0.78	0.21	96,98,100,100	0
55	MG	DA	3147	1/1	0.78	0.22	104,104,104,104	0
55	MG	CA	3134	1/1	0.79	0.28	126,126,126,126	0
55	MG	CA	3073	1/1	0.79	0.19	229,229,229,229	0
61	PEG	DP	201	7/7	0.79	0.20	90,91,93,95	0
55	MG	CA	3001	1/1	0.79	0.29	296,296,296,296	0
55	MG	CA	3021	1/1	0.79	0.39	261,261,261,261	0
55	MG	AA	1626	1/1	0.79	0.21	113,113,113,113	0
55	MG	BA	1647	1/1	0.80	0.19	86,86,86,86	0
55	MG	CA	3137	1/1	0.80	0.18	123,123,123,123	0
55	MG	BA	1640	1/1	0.80	0.35	94,94,94,94	0
55	MG	CA	3014	1/1	0.80	0.16	200,200,200,200	0
58	PUT	AA	1674	6/6	0.80	0.44	128,131,132,133	0
55	MG	BA	1604	1/1	0.81	0.12	187,187,187,187	0
57	MPD	DN	201	8/8	0.81	0.22	84,91,101,101	0
55	MG	CA	3007	1/1	0.81	0.11	214,214,214,214	0
55	MG	CA	3133	1/1	0.81	0.26	83,83,83,83	0
58	PUT	AA	1675	6/6	0.81	0.29	106,107,108,109	0
57	MPD	AA	1676	8/8	0.82	0.35	102,115,118,121	0
55	MG	DA	3111	1/1	0.82	0.38	292,292,292,292	0
55	MG	DA	3133	1/1	0.82	0.19	78,78,78,78	0
55	MG	CA	3115	1/1	0.82	0.27	72,72,72,72	0
55	MG	CA	3150	1/1	0.82	0.15	74,74,74,74	0
55	MG	CA	3028	1/1	0.82	0.13	274,274,274,274	0
55	MG	CA	3068	1/1	0.83	0.14	205,205,205,205	0
55	MG	AA	1601	1/1	0.83	0.55	76,76,76,76	0
55	MG	CA	3113	1/1	0.83	0.54	79,79,79,79	0
55	MG	DA	3130	1/1	0.83	0.38	99,99,99,99	0
55	MG	CA	3131	1/1	0.83	0.17	83,83,83,83	0
55	MG	AA	1608	1/1	0.83	0.32	78,78,78,78	0
55	MG	CA	3120	1/1	0.83	0.19	137,137,137,137	0
55	MG	BA	1623	1/1	0.83	0.24	254,254,254,254	0
55	MG	DA	3176	1/1	0.83	0.29	97,97,97,97	0
55	MG	DA	3180	1/1	0.83	0.22	95,95,95,95	0
55	MG	BA	1648	1/1	0.83	0.25	68,68,68,68	0
67	GUN	DA	3211	11/11	0.83	0.18	82,84,86,86	0
55	MG	CA	3151	1/1	0.84	0.31	81,81,81,81	0
58	PUT	AA	1672	6/6	0.84	0.37	90,93,95,95	0
55	MG	CA	3094	1/1	0.84	0.19	126,126,126,126	0
55	MG	CA	3142	1/1	0.84	0.12	71,71,71,71	0
55	MG	CA	3026	1/1	0.84	0.17	111,111,111,111	0
59	TAC	BA	1643	32/32	0.84	0.14	146,150,152,152	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	PUT	DA	3205	6/6	0.85	0.35	77,82,89,91	0
55	MG	DA	3163	1/1	0.85	0.24	84,84,84,84	0
55	MG	CA	3116	1/1	0.85	0.33	75,75,75,75	0
57	MPD	DT	201	8/8	0.85	0.30	84,87,99,100	0
55	MG	CA	3119	1/1	0.85	0.30	86,86,86,86	0
55	MG	BA	1633	1/1	0.85	0.17	241,241,241,241	0
55	MG	AA	1661	1/1	0.85	0.12	139,139,139,139	0
55	MG	AA	1609	1/1	0.85	0.35	88,88,88,88	0
55	MG	CA	3105	1/1	0.86	0.28	260,260,260,260	0
55	MG	DA	3121	1/1	0.86	0.35	70,70,70,70	0
57	MPD	DA	3190	8/8	0.86	0.17	78,82,85,89	0
55	MG	CA	3109	1/1	0.86	0.15	62,62,62,62	0
55	MG	AA	1611	1/1	0.86	0.30	94,94,94,94	0
55	MG	AA	1655	1/1	0.86	0.08	151,151,151,151	0
55	MG	CA	3128	1/1	0.86	0.12	82,82,82,82	0
55	MG	CA	3062	1/1	0.86	0.10	190,190,190,190	0
58	PUT	DA	3222	6/6	0.86	0.22	41,43,47,47	0
55	MG	CA	3130	1/1	0.86	0.28	76,76,76,76	0
55	MG	CA	3083	1/1	0.86	0.15	203,203,203,203	0
55	MG	CA	3090	1/1	0.86	0.13	170,170,170,170	0
56	PG4	AA	1670	13/13	0.86	0.12	64,79,91,92	0
55	MG	CA	3117	1/1	0.86	0.28	69,69,69,69	0
63	PGE	D1	102	10/10	0.86	0.26	107,117,119,119	0
55	MG	CA	3008	1/1	0.86	0.20	147,147,147,147	0
55	MG	BA	1612	1/1	0.86	0.23	159,159,159,159	0
58	PUT	DA	3195	6/6	0.87	0.30	76,81,86,87	0
55	MG	BA	1630	1/1	0.87	0.14	160,160,160,160	0
57	MPD	DE	302	8/8	0.87	0.31	71,76,83,85	0
55	MG	CA	3093	1/1	0.87	0.10	84,84,84,84	0
55	MG	DA	3062	1/1	0.87	0.14	211,211,211,211	0
55	MG	CA	3138	1/1	0.87	0.20	84,84,84,84	0
55	MG	DA	3173	1/1	0.87	0.32	100,100,100,100	0
55	MG	DA	3120	1/1	0.87	0.30	81,81,81,81	0
55	MG	BA	1616	1/1	0.87	0.19	162,162,162,162	0
55	MG	CA	3010	1/1	0.87	0.19	245,245,245,245	0
55	MG	AA	1605	1/1	0.87	0.45	80,80,80,80	0
55	MG	CA	3080	1/1	0.88	0.16	119,119,119,119	0
55	MG	AA	1604	1/1	0.88	0.23	50,50,50,50	0
55	MG	CA	3108	1/1	0.88	0.21	73,73,73,73	0
55	MG	AA	1618	1/1	0.88	0.57	86,86,86,86	0
61	PEG	D3	101	7/7	0.88	0.53	83,89,94,95	0
57	MPD	DA	3204	8/8	0.88	0.29	117,118,124,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3127	1/1	0.88	0.35	71,71,71,71	0
55	MG	CA	3118	1/1	0.88	0.29	64,64,64,64	0
62	EDO	DA	3198	4/4	0.88	0.26	76,79,79,79	0
55	MG	AA	1606	1/1	0.88	0.33	83,83,83,83	0
55	MG	AA	1623	1/1	0.88	0.11	62,62,62,62	0
66	ACY	DA	3201	4/4	0.88	0.20	66,68,68,69	0
55	MG	CA	3112	1/1	0.88	0.08	62,62,62,62	0
55	MG	CA	3107	1/1	0.89	0.28	65,65,65,65	0
55	MG	AA	1603	1/1	0.89	0.24	81,81,81,81	0
55	MG	AA	1619	1/1	0.89	0.31	93,93,93,93	0
55	MG	CA	3136	1/1	0.89	0.37	87,87,87,87	0
55	MG	CA	3064	1/1	0.89	0.19	260,260,260,260	0
55	MG	AA	1621	1/1	0.89	0.69	97,97,97,97	0
55	MG	BA	1629	1/1	0.89	0.24	184,184,184,184	0
56	PG4	DQ	202	13/13	0.89	0.10	53,59,69,71	0
56	PG4	DR	202	13/13	0.89	0.29	97,109,121,121	0
55	MG	CA	3141	1/1	0.89	0.32	66,66,66,66	0
55	MG	CA	3072	1/1	0.89	0.12	249,249,249,249	0
55	MG	CA	3099	1/1	0.89	0.11	156,156,156,156	0
61	PEG	DA	3226	7/7	0.89	0.20	57,62,74,75	0
55	MG	CA	3022	1/1	0.89	0.24	206,206,206,206	0
55	MG	AA	1615	1/1	0.89	0.48	84,84,84,84	0
55	MG	DA	3138	1/1	0.89	0.56	38,38,38,38	1
63	PGE	DS	201	10/10	0.89	0.14	65,78,83,83	0
63	PGE	DA	3001	10/10	0.89	0.18	75,85,99,101	0
55	MG	DA	3142	1/1	0.89	0.42	84,84,84,84	0
55	MG	CA	3106	1/1	0.89	0.22	75,75,75,75	0
57	MPD	DA	3210	8/8	0.89	0.24	87,89,92,94	0
61	PEG	D1	103	7/7	0.90	0.29	76,77,78,78	0
56	PG4	DA	3193	13/13	0.90	0.21	65,77,93,94	0
55	MG	CA	3126	1/1	0.90	0.29	85,85,85,85	0
55	MG	DA	3171	1/1	0.90	0.09	74,74,74,74	0
55	MG	DA	3141	1/1	0.90	0.12	40,40,40,40	0
62	EDO	DB	211	4/4	0.90	0.31	88,88,90,90	0
62	EDO	DA	3002	4/4	0.90	0.40	71,74,79,82	0
55	MG	CA	3016	1/1	0.90	0.22	164,164,164,164	0
55	MG	CA	3071	1/1	0.90	0.09	152,152,152,152	0
55	MG	DA	3146	1/1	0.90	0.20	70,70,70,70	0
55	MG	CA	3145	1/1	0.90	0.19	62,62,62,62	0
63	PGE	DU	101	10/10	0.90	0.17	79,84,91,92	0
59	TAC	AA	1681	32/32	0.90	0.13	94,106,109,110	0
66	ACY	DA	3191	4/4	0.90	0.21	80,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3137	1/1	0.90	0.35	80,80,80,80	0
57	MPD	DA	3207	8/8	0.90	0.17	86,86,88,89	0
61	PEG	AL	201	7/7	0.90	0.15	79,79,85,86	0
68	TRS	DA	3220	8/8	0.90	0.16	94,100,107,109	0
55	MG	CA	3076	1/1	0.91	0.08	132,132,132,132	0
55	MG	BA	1614	1/1	0.91	0.12	137,137,137,137	0
55	MG	CA	3153	1/1	0.91	0.17	59,59,59,59	0
57	MPD	DT	202	8/8	0.91	0.26	105,107,109,109	0
55	MG	AA	1636	1/1	0.91	0.12	113,113,113,113	0
57	MPD	DA	3192	8/8	0.91	0.23	69,77,79,80	0
55	MG	AA	1664	1/1	0.91	0.10	199,199,199,199	0
55	MG	AA	1625	1/1	0.91	0.16	68,68,68,68	0
56	PG4	DA	3216	13/13	0.91	0.15	77,89,96,96	0
55	MG	DA	3170	1/1	0.91	0.27	90,90,90,90	0
61	PEG	DL	201	7/7	0.91	0.12	66,69,70,71	0
55	MG	CA	3149	1/1	0.91	0.22	63,63,63,63	0
55	MG	CA	3012	1/1	0.91	0.08	84,84,84,84	0
61	PEG	DA	3199	7/7	0.91	0.19	79,84,92,93	0
55	MG	CA	3121	1/1	0.92	0.16	65,65,65,65	0
55	MG	CA	3056	1/1	0.92	0.63	78,78,78,78	0
55	MG	DA	3169	1/1	0.92	0.36	66,66,66,66	0
55	MG	DA	3123	1/1	0.92	0.31	81,81,81,81	0
55	MG	CA	3140	1/1	0.92	0.11	75,75,75,75	0
55	MG	DA	3172	1/1	0.92	0.40	81,81,81,81	0
55	MG	AA	1602	1/1	0.92	0.23	75,75,75,75	0
55	MG	BA	1637	1/1	0.92	0.19	86,86,86,86	0
61	PEG	DA	3227	7/7	0.92	0.21	75,79,86,87	0
55	MG	CA	3143	1/1	0.92	0.07	67,67,67,67	0
55	MG	CA	3037	1/1	0.92	0.21	146,146,146,146	0
56	PG4	BA	1642	13/13	0.92	0.11	84,86,94,96	0
55	MG	AA	1614	1/1	0.92	0.22	79,79,79,79	0
62	EDO	DA	3209	4/4	0.92	0.26	93,94,95,95	0
55	MG	DA	3012	1/1	0.92	0.13	153,153,153,153	0
56	PG4	DS	202	13/13	0.92	0.11	52,54,63,64	0
55	MG	DA	3037	1/1	0.92	0.18	22,22,22,22	0
58	PUT	DA	3212	6/6	0.92	0.19	54,63,66,70	0
63	PGE	DA	3203	10/10	0.92	0.17	68,72,76,76	0
63	PGE	DA	3225	10/10	0.92	0.17	73,81,92,92	0
65	1PE	DA	3202	16/16	0.92	0.17	55,64,72,72	0
55	MG	CA	3039	1/1	0.92	0.10	158,158,158,158	0
59	TAC	AA	1680	32/32	0.92	0.13	70,81,96,96	0
55	MG	BA	1609	1/1	0.92	0.09	168,168,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3152	1/1	0.92	0.42	94,94,94,94	0
55	MG	DA	3158	1/1	0.92	0.18	63,63,63,63	0
55	MG	DA	3129	1/1	0.93	0.34	67,67,67,67	0
55	MG	AA	1630	1/1	0.93	0.11	105,105,105,105	0
55	MG	DA	3131	1/1	0.93	0.26	63,63,63,63	0
62	EDO	DA	3208	4/4	0.93	0.23	69,71,72,72	0
55	MG	AA	1665	1/1	0.93	0.12	136,136,136,136	0
62	EDO	DA	3215	4/4	0.93	0.15	67,71,74,74	0
55	MG	CA	3035	1/1	0.93	0.21	89,89,89,89	0
55	MG	CA	3054	1/1	0.93	0.07	118,118,118,118	0
55	MG	DA	3119	1/1	0.93	0.17	69,69,69,69	0
55	MG	CA	3036	1/1	0.93	0.10	133,133,133,133	0
55	MG	CA	3102	1/1	0.93	0.08	104,104,104,104	0
58	PUT	DA	3188	6/6	0.93	0.13	43,50,50,51	0
64	SPD	DA	3183	10/10	0.93	0.16	60,70,74,75	0
64	SPD	DA	3206	10/10	0.93	0.25	86,93,96,96	0
58	PUT	DA	3189	6/6	0.93	0.14	40,44,47,47	0
55	MG	CA	3078	1/1	0.93	0.10	153,153,153,153	0
61	PEG	DA	3200	7/7	0.93	0.33	65,68,77,77	0
55	MG	DA	3124	1/1	0.93	0.35	76,76,76,76	0
55	MG	AA	1642	1/1	0.93	0.10	89,89,89,89	0
58	PUT	DA	3213	6/6	0.93	0.23	83,85,91,93	0
55	MG	DA	3160	1/1	0.94	0.51	81,81,81,81	0
55	MG	AA	1610	1/1	0.94	0.22	95,95,95,95	0
55	MG	DA	3164	1/1	0.94	0.20	59,59,59,59	0
55	MG	DA	3167	1/1	0.94	0.30	90,90,90,90	0
55	MG	AA	1607	1/1	0.94	0.26	70,70,70,70	0
55	MG	CA	3019	1/1	0.94	0.09	58,58,58,58	0
55	MG	BA	1634	1/1	0.94	0.12	129,129,129,129	0
55	MG	CA	3084	1/1	0.94	0.10	167,167,167,167	0
62	EDO	D1	101	4/4	0.94	0.08	56,57,60,60	0
55	MG	AA	1669	1/1	0.94	0.10	172,172,172,172	0
62	EDO	DB	212	4/4	0.94	0.14	70,72,73,73	0
55	MG	CA	3023	1/1	0.94	0.12	159,159,159,159	0
55	MG	AA	1612	1/1	0.94	0.18	57,57,57,57	0
55	MG	DA	3177	1/1	0.94	0.26	67,67,67,67	0
55	MG	DA	3178	1/1	0.94	0.25	69,69,69,69	0
55	MG	DA	3179	1/1	0.94	0.19	101,101,101,101	0
55	MG	CA	3127	1/1	0.94	0.24	65,65,65,65	0
55	MG	DB	207	1/1	0.94	0.11	80,80,80,80	0
55	MG	DB	209	1/1	0.94	0.20	65,65,65,65	0
55	MG	DB	210	1/1	0.94	0.15	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3114	1/1	0.94	0.14	57,57,57,57	0
58	PUT	DA	3219	6/6	0.94	0.14	63,64,65,66	0
63	PGE	DA	3214	10/10	0.94	0.14	56,58,66,66	0
58	PUT	DA	3221	6/6	0.94	0.20	113,116,117,118	0
55	MG	CA	3048	1/1	0.94	0.08	91,91,91,91	0
58	PUT	DA	3223	6/6	0.94	0.17	54,55,62,64	0
64	SPD	DA	3224	10/10	0.94	0.14	30,40,57,60	0
55	MG	AA	1627	1/1	0.94	0.28	72,72,72,72	0
55	MG	DA	3080	1/1	0.94	0.11	149,149,149,149	0
57	MPD	AA	1671	8/8	0.94	0.21	83,86,89,90	0
55	MG	DA	3149	1/1	0.94	0.06	47,47,47,47	0
55	MG	AA	1679	1/1	0.94	0.24	62,62,62,62	0
55	MG	CA	3058	1/1	0.94	0.21	138,138,138,138	0
62	EDO	DA	3194	4/4	0.95	0.16	61,63,64,65	0
55	MG	DA	3153	1/1	0.95	0.25	53,53,53,53	0
55	MG	DA	3154	1/1	0.95	0.21	62,62,62,62	0
55	MG	BA	1627	1/1	0.95	0.13	126,126,126,126	0
55	MG	CA	3063	1/1	0.95	0.14	118,118,118,118	0
55	MG	DA	3161	1/1	0.95	0.21	62,62,62,62	0
55	MG	CA	3079	1/1	0.95	0.06	116,116,116,116	0
55	MG	DA	3132	1/1	0.95	0.13	54,54,54,54	0
55	MG	DA	3165	1/1	0.95	0.17	47,47,47,47	0
58	PUT	DA	3184	6/6	0.95	0.15	53,55,60,60	0
55	MG	AA	1634	1/1	0.95	0.09	144,144,144,144	0
55	MG	CA	3082	1/1	0.95	0.16	112,112,112,112	0
55	MG	BA	1617	1/1	0.95	0.06	105,105,105,105	0
61	PEG	DA	3218	7/7	0.95	0.21	99,105,110,112	0
55	MG	AA	1656	1/1	0.95	0.08	140,140,140,140	0
65	1PE	DA	3185	16/16	0.95	0.11	37,52,80,82	0
55	MG	CA	3055	1/1	0.95	0.07	135,135,135,135	0
55	MG	AA	1663	1/1	0.95	0.06	94,94,94,94	0
55	MG	BA	1645	1/1	0.95	0.10	94,94,94,94	0
55	MG	CA	3074	1/1	0.95	0.07	101,101,101,101	0
55	MG	BA	1635	1/1	0.95	0.09	113,113,113,113	0
55	MG	AA	1658	1/1	0.95	0.12	101,101,101,101	0
62	EDO	DB	201	4/4	0.96	0.16	72,75,76,76	0
55	MG	CB	202	1/1	0.96	0.11	113,113,113,113	0
55	MG	CB	203	1/1	0.96	0.07	133,133,133,133	0
55	MG	DA	3117	1/1	0.96	0.27	62,62,62,62	0
55	MG	BA	1619	1/1	0.96	0.07	79,79,79,79	0
55	MG	CA	3088	1/1	0.96	0.06	67,67,67,67	0
62	EDO	DA	3197	4/4	0.96	0.09	51,51,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3046	1/1	0.96	0.10	117,117,117,117	0
55	MG	CA	3092	1/1	0.96	0.06	125,125,125,125	0
55	MG	CA	3024	1/1	0.96	0.10	81,81,81,81	0
55	MG	DA	3125	1/1	0.96	0.30	58,58,58,58	0
55	MG	DA	3126	1/1	0.96	0.32	57,57,57,57	0
55	MG	CA	3011	1/1	0.96	0.06	70,70,70,70	0
55	MG	CA	3049	1/1	0.96	0.05	57,57,57,57	0
55	MG	CA	3053	1/1	0.96	0.10	81,81,81,81	0
63	PGE	DA	3186	10/10	0.96	0.09	33,40,41,41	0
60	ZN	C5	101	1/1	0.96	0.07	149,149,149,149	0
55	MG	AA	1633	1/1	0.96	0.06	128,128,128,128	0
63	PGE	DA	3217	10/10	0.96	0.15	67,71,76,76	0
55	MG	DR	203	1/1	0.96	0.13	140,140,140,140	0
55	MG	CA	3031	1/1	0.96	0.06	73,73,73,73	0
55	MG	DB	208	1/1	0.96	0.09	77,77,77,77	0
55	MG	AA	1657	1/1	0.96	0.10	105,105,105,105	0
55	MG	DA	3175	1/1	0.96	0.14	68,68,68,68	0
55	MG	DA	3140	1/1	0.96	0.17	68,68,68,68	0
55	MG	CA	3057	1/1	0.96	0.07	106,106,106,106	0
55	MG	AA	1647	1/1	0.96	0.09	149,149,149,149	0
55	MG	DA	3143	1/1	0.96	0.11	50,50,50,50	0
55	MG	CA	3018	1/1	0.96	0.07	90,90,90,90	0
55	MG	CB	201	1/1	0.96	0.06	159,159,159,159	0
55	MG	DA	3095	1/1	0.97	0.09	74,74,74,74	0
55	MG	AA	1613	1/1	0.97	0.35	59,59,59,59	0
55	MG	CA	3051	1/1	0.97	0.04	73,73,73,73	0
55	MG	CA	3066	1/1	0.97	0.08	110,110,110,110	0
55	MG	DA	3145	1/1	0.97	0.11	78,78,78,78	0
55	MG	CA	3025	1/1	0.97	0.05	87,87,87,87	0
55	MG	CA	3006	1/1	0.97	0.07	143,143,143,143	0
55	MG	DA	3181	1/1	0.97	0.21	70,70,70,70	0
55	MG	DA	3148	1/1	0.97	0.30	62,62,62,62	0
55	MG	CA	3069	1/1	0.97	0.09	110,110,110,110	0
55	MG	DA	3151	1/1	0.97	0.14	30,30,30,30	0
55	MG	CA	3070	1/1	0.97	0.04	87,87,87,87	0
55	MG	DB	206	1/1	0.97	0.16	64,64,64,64	0
55	MG	CA	3089	1/1	0.97	0.13	54,54,54,54	0
55	MG	DA	3155	1/1	0.97	0.27	60,60,60,60	0
55	MG	DA	3156	1/1	0.97	0.25	72,72,72,72	0
55	MG	DA	3157	1/1	0.97	0.21	54,54,54,54	0
55	MG	CA	3020	1/1	0.97	0.07	86,86,86,86	0
55	MG	DA	3128	1/1	0.97	0.52	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3029	1/1	0.97	0.17	114,114,114,114	0
55	MG	DA	3162	1/1	0.97	0.11	57,57,57,57	0
55	MG	CA	3042	1/1	0.97	0.06	82,82,82,82	0
55	MG	CA	3043	1/1	0.97	0.07	86,86,86,86	0
55	MG	AA	1620	1/1	0.97	0.16	63,63,63,63	0
55	MG	DA	3043	1/1	0.97	0.09	32,32,32,32	0
55	MG	DA	3134	1/1	0.97	0.15	95,95,95,95	0
55	MG	DA	3044	1/1	0.97	0.06	70,70,70,70	0
55	MG	BA	1605	1/1	0.97	0.05	146,146,146,146	0
55	MG	DA	3139	1/1	0.97	0.08	55,55,55,55	0
55	MG	BA	1601	1/1	0.97	0.09	130,130,130,130	0
55	MG	CA	3065	1/1	0.98	0.07	72,72,72,72	0
55	MG	DA	3079	1/1	0.98	0.04	124,124,124,124	0
55	MG	CA	3085	1/1	0.98	0.04	69,69,69,69	0
55	MG	DA	3082	1/1	0.98	0.05	72,72,72,72	0
55	MG	CA	3086	1/1	0.98	0.06	59,59,59,59	0
55	MG	AA	1651	1/1	0.98	0.05	69,69,69,69	0
55	MG	CA	3144	1/1	0.98	0.03	63,63,63,63	0
55	MG	CA	3027	1/1	0.98	0.06	68,68,68,68	0
55	MG	AA	1635	1/1	0.98	0.09	104,104,104,104	0
55	MG	CA	3091	1/1	0.98	0.06	80,80,80,80	0
57	MPD	DS	203	8/8	0.98	0.14	47,50,57,58	0
55	MG	DA	3122	1/1	0.98	0.27	46,46,46,46	0
55	MG	CA	3013	1/1	0.98	0.06	99,99,99,99	0
55	MG	CA	3030	1/1	0.98	0.05	64,64,64,64	0
55	MG	CA	3052	1/1	0.98	0.06	71,71,71,71	0
55	MG	CA	3095	1/1	0.98	0.04	69,69,69,69	0
55	MG	CA	3098	1/1	0.98	0.04	78,78,78,78	0
55	MG	BA	1608	1/1	0.98	0.05	86,86,86,86	0
55	MG	DA	3166	1/1	0.98	0.11	88,88,88,88	0
55	MG	CA	3101	1/1	0.98	0.04	97,97,97,97	0
55	MG	AA	1659	1/1	0.98	0.05	74,74,74,74	0
55	MG	CA	3103	1/1	0.98	0.04	90,90,90,90	0
58	PUT	DM	201	6/6	0.98	0.10	40,48,52,56	0
55	MG	BA	1610	1/1	0.98	0.06	93,93,93,93	0
55	MG	BA	1626	1/1	0.98	0.04	85,85,85,85	0
55	MG	AA	1668	1/1	0.98	0.10	59,59,59,59	0
55	MG	DA	3136	1/1	0.98	0.09	43,43,43,43	0
55	MG	BA	1628	1/1	0.98	0.04	92,92,92,92	0
55	MG	BA	1613	1/1	0.98	0.10	79,79,79,79	0
55	MG	AA	1644	1/1	0.98	0.15	87,87,87,87	0
55	MG	DA	3008	1/1	0.98	0.07	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1632	1/1	0.98	0.10	78,78,78,78	0
64	SPD	DA	3187	10/10	0.98	0.09	30,41,47,48	0
55	MG	DA	3015	1/1	0.98	0.05	40,40,40,40	0
55	MG	DA	3026	1/1	0.98	0.06	92,92,92,92	0
55	MG	DA	3182	1/1	0.98	0.22	52,52,52,52	0
55	MG	DA	3230	1/1	0.98	0.06	48,48,48,48	0
55	MG	DA	3231	1/1	0.98	0.13	36,36,36,36	0
55	MG	CA	3081	1/1	0.98	0.04	84,84,84,84	0
60	ZN	AB	301	1/1	0.98	0.06	150,150,150,150	0
55	MG	AA	1641	1/1	0.98	0.06	65,65,65,65	0
55	MG	CA	3045	1/1	0.98	0.07	107,107,107,107	0
55	MG	DA	3064	1/1	0.99	0.11	49,49,49,49	0
55	MG	DA	3070	1/1	0.99	0.04	62,62,62,62	0
55	MG	DA	3072	1/1	0.99	0.07	55,55,55,55	0
55	MG	DA	3159	1/1	0.99	0.06	76,76,76,76	0
55	MG	DA	3074	1/1	0.99	0.05	47,47,47,47	0
55	MG	DA	3078	1/1	0.99	0.05	52,52,52,52	0
55	MG	BA	1602	1/1	0.99	0.05	84,84,84,84	0
55	MG	CA	3040	1/1	0.99	0.04	83,83,83,83	0
55	MG	BA	1631	1/1	0.99	0.03	45,45,45,45	0
55	MG	DA	3083	1/1	0.99	0.05	45,45,45,45	0
55	MG	DA	3085	1/1	0.99	0.03	50,50,50,50	0
55	MG	BA	1615	1/1	0.99	0.04	65,65,65,65	0
55	MG	DA	3098	1/1	0.99	0.06	87,87,87,87	0
55	MG	DA	3101	1/1	0.99	0.03	45,45,45,45	0
55	MG	CA	3044	1/1	0.99	0.07	59,59,59,59	0
60	ZN	D5	101	1/1	0.99	0.02	55,55,55,55	0
55	MG	DA	3113	1/1	0.99	0.06	52,52,52,52	0
55	MG	DA	3114	1/1	0.99	0.04	39,39,39,39	0
55	MG	AA	1639	1/1	0.99	0.04	89,89,89,89	0
55	MG	DA	3174	1/1	0.99	0.07	70,70,70,70	0
55	MG	DA	3118	1/1	0.99	0.07	36,36,36,36	0
55	MG	AA	1645	1/1	0.99	0.04	46,46,46,46	0
55	MG	CA	3096	1/1	0.99	0.02	64,64,64,64	0
55	MG	CA	3004	1/1	0.99	0.06	106,106,106,106	0
55	MG	BA	1618	1/1	0.99	0.03	69,69,69,69	0
55	MG	CA	3100	1/1	0.99	0.07	73,73,73,73	0
55	MG	AA	1629	1/1	0.99	0.04	71,71,71,71	0
55	MG	CA	3050	1/1	0.99	0.03	54,54,54,54	0
55	MG	DA	3228	1/1	0.99	0.07	36,36,36,36	0
55	MG	DR	201	1/1	0.99	0.08	32,32,32,32	0
55	MG	BA	1620	1/1	0.99	0.04	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	202	1/1	0.99	0.07	52,52,52,52	0
55	MG	DB	204	1/1	0.99	0.04	37,37,37,37	0
55	MG	BA	1621	1/1	0.99	0.14	36,36,36,36	0
55	MG	BA	1622	1/1	0.99	0.06	99,99,99,99	0
55	MG	AA	1667	1/1	0.99	0.07	41,41,41,41	0
55	MG	AA	1648	1/1	0.99	0.04	60,60,60,60	0
55	MG	AA	1649	1/1	0.99	0.04	57,57,57,57	0
55	MG	DA	3135	1/1	0.99	0.04	78,78,78,78	0
55	MG	DA	3006	1/1	0.99	0.04	75,75,75,75	0
55	MG	DA	3007	1/1	0.99	0.06	88,88,88,88	0
55	MG	CA	3033	1/1	0.99	0.11	91,91,91,91	0
55	MG	AA	1650	1/1	0.99	0.03	79,79,79,79	0
55	MG	CA	3059	1/1	0.99	0.03	74,74,74,74	0
55	MG	DA	3016	1/1	0.99	0.05	43,43,43,43	0
55	MG	AA	1638	1/1	0.99	0.04	86,86,86,86	0
55	MG	DA	3028	1/1	0.99	0.04	56,56,56,56	0
55	MG	DA	3030	1/1	0.99	0.04	42,42,42,42	0
55	MG	DA	3035	1/1	0.99	0.08	32,32,32,32	0
55	MG	AA	1653	1/1	0.99	0.05	61,61,61,61	0
55	MG	CA	3017	1/1	0.99	0.07	75,75,75,75	0
55	MG	CA	3087	1/1	0.99	0.03	59,59,59,59	0
55	MG	DA	3047	1/1	0.99	0.06	58,58,58,58	0
55	MG	DA	3150	1/1	0.99	0.05	50,50,50,50	0
55	MG	DA	3049	1/1	0.99	0.03	39,39,39,39	0
55	MG	DA	3052	1/1	0.99	0.03	70,70,70,70	0
55	MG	DA	3054	1/1	0.99	0.05	70,70,70,70	0
55	MG	AA	1662	1/1	0.99	0.04	73,73,73,73	0
55	MG	DA	3063	1/1	0.99	0.04	85,85,85,85	0
55	MG	CA	3097	1/1	1.00	0.05	83,83,83,83	0
55	MG	DA	3086	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3087	1/1	1.00	0.01	34,34,34,34	0
55	MG	DA	3088	1/1	1.00	0.02	42,42,42,42	0
55	MG	DA	3089	1/1	1.00	0.04	23,23,23,23	0
55	MG	DA	3229	1/1	1.00	0.04	36,36,36,36	0
55	MG	DA	3090	1/1	1.00	0.04	30,30,30,30	0
55	MG	DA	3091	1/1	1.00	0.05	17,17,17,17	0
55	MG	DA	3092	1/1	1.00	0.02	21,21,21,21	0
55	MG	DA	3093	1/1	1.00	0.07	23,23,23,23	0
55	MG	DA	3094	1/1	1.00	0.07	20,20,20,20	0
55	MG	DA	3017	1/1	1.00	0.01	20,20,20,20	0
55	MG	DA	3096	1/1	1.00	0.05	36,36,36,36	0
55	MG	DA	3097	1/1	1.00	0.03	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3018	1/1	1.00	0.02	43,43,43,43	0
55	MG	DA	3099	1/1	1.00	0.04	23,23,23,23	0
55	MG	DA	3100	1/1	1.00	0.02	26,26,26,26	0
55	MG	DA	3019	1/1	1.00	0.15	8,8,8,8	0
55	MG	DA	3102	1/1	1.00	0.02	30,30,30,30	0
55	MG	DA	3103	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3104	1/1	1.00	0.05	34,34,34,34	0
55	MG	DA	3105	1/1	1.00	0.07	31,31,31,31	0
55	MG	DA	3106	1/1	1.00	0.10	41,41,41,41	0
55	MG	DA	3107	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3108	1/1	1.00	0.05	30,30,30,30	0
55	MG	DA	3109	1/1	1.00	0.02	23,23,23,23	0
55	MG	DA	3110	1/1	1.00	0.05	35,35,35,35	0
55	MG	DA	3020	1/1	1.00	0.04	45,45,45,45	0
55	MG	DA	3112	1/1	1.00	0.04	24,24,24,24	0
55	MG	DA	3021	1/1	1.00	0.04	27,27,27,27	0
55	MG	DA	3022	1/1	1.00	0.07	21,21,21,21	0
55	MG	DA	3115	1/1	1.00	0.02	37,37,37,37	0
55	MG	DA	3116	1/1	1.00	0.02	34,34,34,34	0
55	MG	DA	3023	1/1	1.00	0.04	20,20,20,20	0
55	MG	DA	3024	1/1	1.00	0.07	36,36,36,36	0
55	MG	DA	3025	1/1	1.00	0.02	31,31,31,31	0
55	MG	AA	1637	1/1	1.00	0.04	53,53,53,53	0
55	MG	DA	3027	1/1	1.00	0.03	33,33,33,33	0
55	MG	AA	1631	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3029	1/1	1.00	0.10	29,29,29,29	0
55	MG	DB	203	1/1	1.00	0.03	30,30,30,30	0
55	MG	DA	3031	1/1	1.00	0.02	27,27,27,27	0
55	MG	DA	3032	1/1	1.00	0.06	23,23,23,23	0
55	MG	DA	3033	1/1	1.00	0.05	26,26,26,26	0
55	MG	DA	3034	1/1	1.00	0.02	16,16,16,16	0
55	MG	AA	1643	1/1	1.00	0.02	53,53,53,53	0
55	MG	DA	3036	1/1	1.00	0.06	25,25,25,25	0
55	MG	DB	205	1/1	1.00	0.03	46,46,46,46	0
55	MG	DA	3038	1/1	1.00	0.01	19,19,19,19	0
55	MG	DA	3039	1/1	1.00	0.05	23,23,23,23	0
55	MG	DA	3040	1/1	1.00	0.04	36,36,36,36	0
55	MG	DA	3041	1/1	1.00	0.12	11,11,11,11	0
55	MG	DA	3042	1/1	1.00	0.03	29,29,29,29	0
55	MG	AA	1632	1/1	1.00	0.02	65,65,65,65	0
55	MG	CA	3015	1/1	1.00	0.13	57,57,57,57	0
55	MG	DA	3045	1/1	1.00	0.04	49,49,49,49	0

Continued on next page...

Continued from previous page...

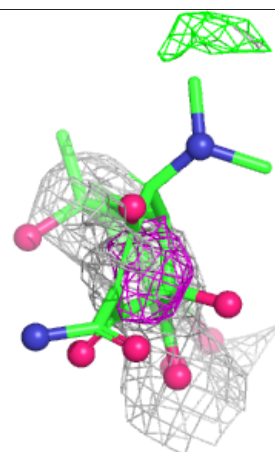
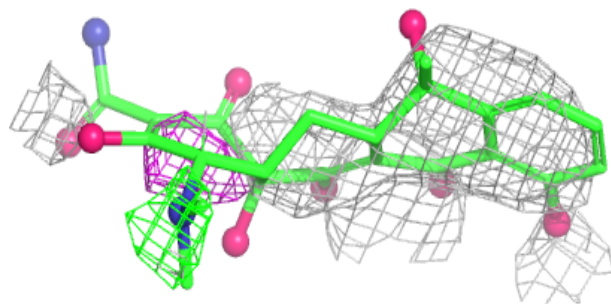
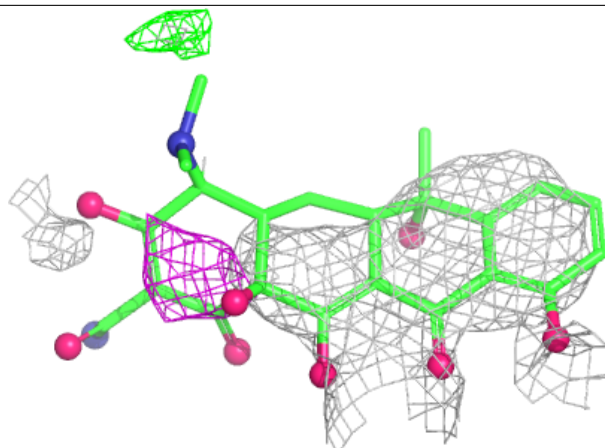
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3046	1/1	1.00	0.03	31,31,31,31	0
55	MG	AA	1640	1/1	1.00	0.05	52,52,52,52	0
55	MG	DA	3048	1/1	1.00	0.03	26,26,26,26	0
55	MG	AA	1666	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3050	1/1	1.00	0.02	18,18,18,18	0
55	MG	DA	3051	1/1	1.00	0.02	14,14,14,14	0
55	MG	BA	1611	1/1	1.00	0.04	56,56,56,56	0
55	MG	DA	3053	1/1	1.00	0.04	44,44,44,44	0
55	MG	DA	3004	1/1	1.00	0.03	60,60,60,60	0
55	MG	DA	3055	1/1	1.00	0.06	24,24,24,24	0
55	MG	DA	3056	1/1	1.00	0.03	42,42,42,42	0
55	MG	DA	3057	1/1	1.00	0.03	13,13,13,13	0
55	MG	DA	3058	1/1	1.00	0.02	32,32,32,32	0
55	MG	DA	3059	1/1	1.00	0.01	23,23,23,23	0
55	MG	DA	3060	1/1	1.00	0.04	21,21,21,21	0
55	MG	DA	3061	1/1	1.00	0.03	30,30,30,30	0
55	MG	DA	3005	1/1	1.00	0.07	60,60,60,60	0
55	MG	AA	1652	1/1	1.00	0.14	21,21,21,21	0
55	MG	AA	1646	1/1	1.00	0.02	49,49,49,49	0
55	MG	DA	3065	1/1	1.00	0.03	19,19,19,19	0
55	MG	DA	3066	1/1	1.00	0.07	40,40,40,40	0
55	MG	DA	3067	1/1	1.00	0.03	36,36,36,36	0
55	MG	DA	3068	1/1	1.00	0.05	35,35,35,35	0
55	MG	DA	3069	1/1	1.00	0.09	46,46,46,46	0
55	MG	CA	3041	1/1	1.00	0.04	50,50,50,50	0
55	MG	DA	3071	1/1	1.00	0.07	34,34,34,34	0
55	MG	DA	3009	1/1	1.00	0.03	23,23,23,23	0
55	MG	DA	3073	1/1	1.00	0.01	31,31,31,31	0
55	MG	DA	3010	1/1	1.00	0.04	17,17,17,17	0
55	MG	DA	3075	1/1	1.00	0.04	37,37,37,37	0
55	MG	DA	3076	1/1	1.00	0.02	23,23,23,23	0
55	MG	DA	3077	1/1	1.00	0.01	30,30,30,30	0
55	MG	DA	3011	1/1	1.00	0.02	33,33,33,33	0
55	MG	DD	301	1/1	1.00	0.04	40,40,40,40	0
55	MG	DA	3013	1/1	1.00	0.04	19,19,19,19	0
55	MG	DA	3081	1/1	1.00	0.04	45,45,45,45	0
55	MG	DA	3014	1/1	1.00	0.02	14,14,14,14	0
55	MG	DM	202	1/1	1.00	0.05	34,34,34,34	0
55	MG	DA	3084	1/1	1.00	0.06	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

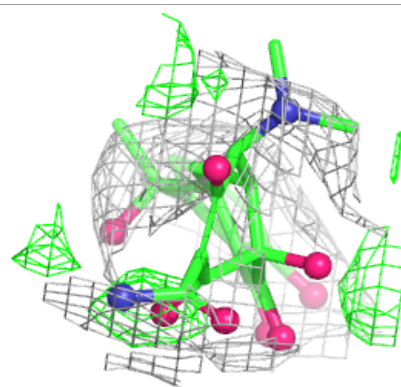
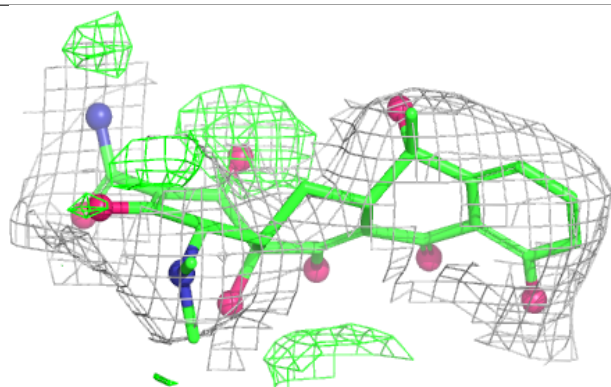
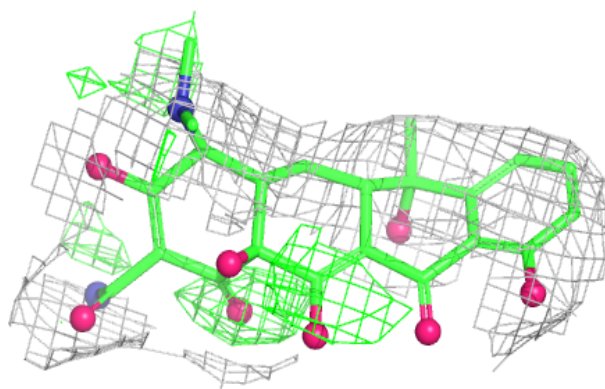
Electron density around TAC BA 1644:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

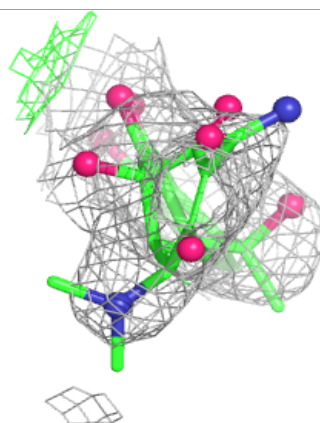
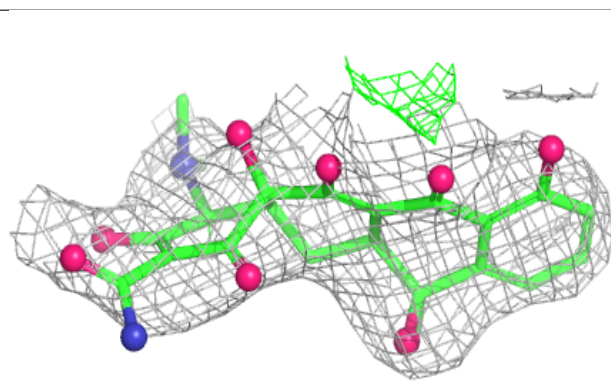
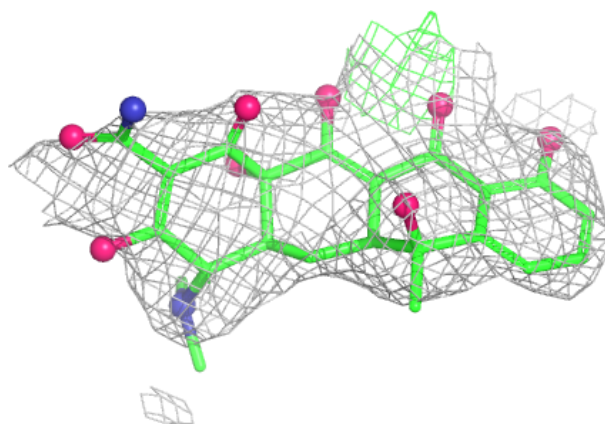


Electron density around TAC BA 1643:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

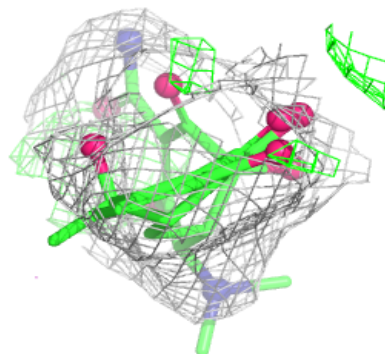
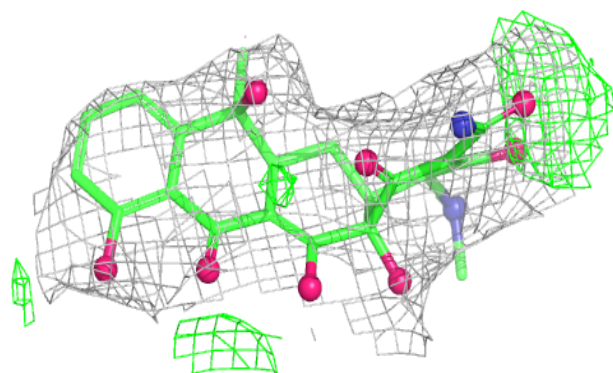
**Electron density around TAC AA 1681:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TAC AA 1680:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.